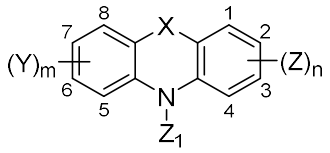
CLAIMS

1. A compound of Formula I:



(I),

or a pharmaceutically acceptable salt or ester thereof, wherein

X is $C(R_X)_2$, O, S, CH=CH, or absent;

each R_X is independently H, CH_3, CF_3, CF_2H, or F, or two R_X together form =O, $=CH_2$, or $=CF_2$, or two R_X, together with the carbon atom to which they are bonded, form a cyclopropyl;

Z_1 is $(C(R_Z)_2)_p$-T_1;

p is 1, 2, 3, 4, 5, or 6;

each R_Z is independently H, C_1-C_4 alkyl, C_1-C_4 alkyl substituted with one or more halogen, or halogen;

T_1 is ~~CHOR$_1$,~~ $C(O)R_1$, $C(O)OR_1$, $C(O)N(R_1)_2$, $NR_1C(O)R_1$, $C(S)R_1$, $C(S)N(R_1)_2$, $NR_1C(S)R_1$, $C(O)NHS(O)_2R_S$, $C(O)NHCOR_1$, C(O)NHOH, or C(O)NHCN;

R_S is R_1, C_3-C_8 cycloalkyl, heterocyclyl comprising one 5- or 6-membered rings and 1-2 heteroatoms selected from N, O, and S, or C_6-C_{10} aryl, wherein the cycloalkyl, heterocyclyl, or aryl is optionally substituted with one or more groups independently selected from C_1-C_4 alkyl;

each R_1 is independently H, C_1-C_4 alkyl, or C_1-C_4 alkyl substituted with one or more halogen;

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

each Y is independently C_1-C_6 alkyl, C_2-C_6 alkenyl, C_2-C_6 alkynyl, halogen, CN, OH, O-(C_1-C_6 alkyl), S-(C_1-C_6 alkyl), O-(C_2-C_4 alkenyl), O-(C_2-C_4 alkynyl), NH_2, NH-C_1-C_6 alkyl, N-(C_1-C_6 alkyl)$_2$, S(O)-(C_1-C_6 alkyl), $S(O)_2$-(C_1-C_6 alkyl), or Q-T, wherein the alkyl, alkenyl, or alkynyl moiety is optionally substituted with one or more groups independently selected from OH, NH_2, N_3, halogen, O-(C_1-C_6 alkyl), S-(C_1-C_6 alkyl), NH-C_1-C_6 alkyl, and N-(C_1-C_6 alkyl)$_2$, or two Y, together with the two adjacent carbon atoms to which they are bonded, form a 5- to 7-membered carbocycle or phenyl;

n is ~~0, 1,~~ 2, 3, or 4;

each Z is independently C_1-C_6 alkyl, C_2-C_6 alkenyl, C_2-C_6 alkynyl, halogen, ~~CN,~~ OH, O-(C_1-C_6 alkyl), S-(C_1-C_6 alkyl), O-(C_2-C_4 alkenyl), O-(C_2-C_4 alkynyl), NH_2, NH-C_1-C_6

alkyl, N-(C_1-C_6 alkyl)$_2$, S(O)-(C_1-C_6 alkyl), S(O)$_2$-(C_1-C_6 alkyl), or Q-T, wherein the alkyl, alkenyl, or alkynyl moiety is optionally substituted with one or more groups independently selected from OH, NH_2, N_3, halogen, O-(C_1-C_6 alkyl), S-(C_1-C_6 alkyl), NH-C_1-C_6 alkyl, and N-(C_1-C_6 alkyl)$_2$;

each Q is independently a bond, NH, N(C_1-C_3 alkyl), O, S, S(O), S(O)$_2$, Q', NH-Q', N(C_1-C_3 alkyl)-Q', O-Q', S-Q', S(O)-Q', or S(O)$_2$-Q';

each Q' is independently a carbon linker comprising one or more C(R_Q)$_2$, C(R_Q)$_2$-C(R_Q)$_2$, CR_Q=CR_Q, or C≡C;

each R_Q is independently H or C_1-C_3 alkyl;

each T is independently C(O)-C_1-C_6 alkyl, C(O)O-C_1-C_6 alkyl, C_3-C_8 cycloalkyl, C_3-C_8 cycloalkenyl, heterocyclyl comprising one or two 5- or 6-membered rings and 1-4 heteroatoms selected from N, O, and S, C_6-C_{10} aryl, or heteroaryl comprising one or two 5- or 6-membered rings and 1-4 heteroatoms selected from N, O, and S, wherein the cycloalkyl, cycloalkenyl, heterocyclyl, aryl, or heteroaryl is optionally substituted with one or more R_T;

each R_T is independently C_1-C_6 alkyl, C_1-C_6 haloalkyl, OH, CN, halogen, O-(C_1-C_6 alkyl), O-(C_1-C_6 haloalkyl), S-(C_1-C_6 alkyl), NH_2, NH-C_1-C_6 alkyl, N-(C_1-C_6 alkyl)$_2$, NHS(O)$_2$-(C_1-C_6 alkyl), (CH_2)$_q$-C_3-C_8 cycloalkyl, (CH_2)$_q$-heterocyclyl, (CH_2)$_q$-phenyl, or (CH_2)$_q$-heteroaryl, wherein the heterocyclyl or heteroaryl comprises one or two 5- or 6-membered rings and 1-4 heteroatoms selected from N, O, and S; and

q is 0, 1, 2, or 3, and

wherein the compound of Formula I is substituted with Z at least at the 3-position and the 4-position, and when X is ~~C(O)~~S or =CH_2 then T is not C(O)R_1 or C(O)OR_1. ~~and each R_Z is H:~~

~~m and n are not both 0; and~~

~~the compound of Formula I is not mono-substituted at the 2- or 7-position with Cl; and~~

~~the compound of Formula I is not di-substituted at the 2- and 8-positions or at the 1- and 7-positions with halogens selected from F and Cl.~~

2. The compound of claim 1, wherein X is C(R_X)$_2$.

3. The compound of claim 1 or 2, wherein each R_X is H, or ~~.~~

~~4. The compound of claim 1 or 2, wherein at least one R_X is CH_3, CF_3, CF_2H, or F.~~

~~5. The compound of claim 1 or 2,~~ wherein two R_X together form =O, $=CH_2$, or $=CF_2$.

4<u>6</u>. The compound of claim ~~1 or 2~~3, wherein two R_X, together ~~with the carbon atom to which they are bonded, form a cyclopropyl.~~<u>form =O.</u>

~~7. The compound of claim 1, wherein X is O.~~

~~8. The compound of claim 1, wherein X is S.~~

~~9. The compound of claim 1, wherein X is CH=CH.~~

~~10. The compound of claim 1, wherein X is absent.~~

~~11. The compound of any one of claims 1-10, wherein p is 1, 2, or 3.~~

~~12. The compound of any one of claims 1-11, wherein p is 1 or 2.~~

~~13. The compound of any one of claims 1-12, wherein p is 1.~~

~~14. The compound of any one of claims 1-10, wherein p is 2, 3, 4, 5, or 6.~~

~~15. The compound of any one of claims 1-14, wherein each R_Z is H.~~

~~1~~6<u>5</u>. The compound of any one of claims 1-~~1~~4, wherein <u>each</u> ~~at least one~~ R_Z is C_1-C_4 alkyl, C_1-C_4 alkyl substituted with one or more halogen, or halogen.

~~1~~7<u>6</u>. The compound of any one of claims 1-~~1~~6<u>5</u>, wherein T_1 is ~~$CHOR_1$,~~ $C(O)R_1$, $C(O)OR_1$, $C(O)N(R_1)_2$, or $NR_1C(O)R_1$.

~~1~~8<u>7</u>. The compound of any one of claims 1-~~1~~6<u>6</u>, wherein T_1 is $C(O)OR_1$, $C(O)N(R_1)_2$, $C(O)NHS(O)_2R_S$, $C(O)NHCOR_1$, C(O)NHOH, or C(O)NHCN.

~~198~~. The compound of any one of claims 1-~~187~~, wherein each R_1 is H.

~~20. The compound of any one of claims 1-18, wherein at least one R_1 is C_1-C_4 alkyl, or C_1-C_4 alkyl substituted with one or more halogen.~~

~~219~~. The compound of any one of claims 1-~~208~~, wherein m is 0 or 1.

~~22. The compound of any one of claims 1-20, wherein m is 1 or 2.~~

~~2310~~. The compound of any one of claims 1-~~920 and 22~~, wherein at least one Y is C_1-C_6 alkyl, C_2-C_6 alkenyl, C_2-C_6 alkynyl, halogen, OH, O-(C_1-C_6 alkyl), O-(C_2-C_4 alkenyl), O-(C_2-C_4 alkynyl), S-(C_1-C_6 alkyl), S(O)-(C_1-C_6 alkyl), S(O)$_2$-(C_1-C_6 alkyl), NH_2, NH-C_1-C_6 alkyl, N-(C_1-C_6 alkyl)$_2$, or Q-T, wherein the alkyl, alkenyl, or alkynyl is optionally substituted with one or more groups independently selected from OH, NH_2, N_3, halogen, O-(C_1-C_6 alkyl), S-(C_1-C_6 alkyl), NH-C_1-C_6 alkyl, and N-(C_1-C_6 alkyl)$_2$ or ~~.~~

~~24. The compound of any one of claims 1-20, 22, and 23, wherein at least one Y is Q-T, C_1-C_6 alkyl, halogen, OH, O-(C_1-C_6 alkyl), O-(C_2-C_4 alkenyl), O-(C_2-C_4 alkynyl), S-(C_1-C_6 alkyl), S(O)-(C_1-C_6 alkyl), S(O)$_2$-(C_1-C_6 alkyl), NH_2, NH-C_1-C_6 alkyl, or N-(C_1-C_6 alkyl)$_2$.~~

~~25. The compound of any one of claims 1-20 and 22,~~ wherein two Y, together with the two adjacent carbon atoms to which they are bonded, form a cyclopentyl, cyclohexyl, cycloheptyl, cyclopentenyl, cyclohexenyl, cycloheptenyl, cyclopentynyl, cyclohexynyl, or cycloheptynyl.

~~26. The compound of any one of claims 1-20 and 22, wherein two Y, together with the two adjacent carbon atoms to which they are bonded, form phenyl.~~

~~27. The compound of any one of claims 1-24, wherein at least one Y is at the 5-position in Formula I.~~

~~28. The compound of any one of claims 1-24, wherein at least one Y is at the 6-position in Formula I.~~

~~29. The compound of any one of claims 1-24, wherein at least one Y is at the 7-position in Formula I.~~

~~30. The compound of any one of claims 1-24, wherein at least one Y is at the 5-position and at least one Y is at the 6-position in Formula I.~~

~~31. The compound of any one of claims 1-24, wherein at least one Y is at the 7-position and at least one Y is at the 6-position in Formula I.~~

~~32. The compound of any one of claims 1-31, wherein n is 0.~~

~~33. The compound of any one of claims 1-31, wherein n is 1 or 2.~~

~~34. The compound of any one of claims 1-31 and 33, wherein at least one Z is C_1-C_6 alkyl, C_2-C_6 alkenyl, C_2-C_6 alkynyl, halogen, CN, OH, O-(C_1-C_6 alkyl), O-(C_2-C_4 alkenyl), O-(C_2-C_4 alkynyl), S-(C_1-C_6 alkyl), S(O)-(C_1-C_6 alkyl), S(O)$_2$-(C_1-C_6 alkyl), NH_2, NH-C_1-C_6 alkyl, N-(C_1-C_6 alkyl)$_2$, or Q-T, wherein the alkyl, alkenyl, or alkynyl is optionally substituted with one or more groups independently selected from OH, NH_2, N_3, halogen, O-(C_1-C_6 alkyl), S-(C_1-C_6 alkyl), NH-C_1-C_6 alkyl, and N-(C_1-C_6 alkyl)$_2$.~~

~~35~~11. The compound of any one of claims 1-31, 33, and 34, wherein at least one Z is Q-T, C_1-C_6 alkyl, halogen, ~~CN,~~ OH, O-(C_1-C_6 alkyl), O-(C_2-C_4 alkenyl), O-(C_2-C_4 alkynyl), S-(C_1-C_6 alkyl), S(O)-(C_1-C_6 alkyl), S(O)$_2$-(C_1-C_6 alkyl), NH_2, NH-C_1-C_6 alkyl, or N-(C_1-C_6 alkyl)$_2$.

~~36. The compound of any one of claims 1-31, 33, and 34, wherein at least one Z is C_1-C_6 alkyl, halogen, CN, OH, O-(C_1-C_6 alkyl), O-(C_2-C_4 alkenyl), O-(C_2-C_4 alkynyl), S-(C_1-C_6 alkyl), S(O)-(C_1-C_6 alkyl), S(O)$_2$-(C_1-C_6 alkyl), NH_2, NH-C_1-C_6 alkyl, or N-(C_1-C_6 alkyl)$_2$.~~

~~37~~12. The compound of any one of claims 1-31 and 33-36, wherein at least one Z is halogen.

~~38. The compound of any one of claims 1-31 and 33-37, wherein at least one Z is Cl or Br.~~

~~39. The compound of any one of claims 1-31 and 33-38, wherein each Z is Cl.~~

~~40. The compound of any one of claims 1-31 and 33-38, wherein each Z is Br.~~

~~41. The compound of any one of claims 1-31 and 33-38, wherein one Z is Cl, and the other Z is Br.~~

~~42. The compound of any one of claims 1-31 and 33-41, wherein at least one Z is at the 3-position in Formula I.~~

~~43. The compound of any one of claims 1-31 and 33-41, wherein at least one Z is at the 4-position.~~

~~44. The compound of any one of claims 1-31 and 33-41, wherein at least one Z is at the 3-position and at least one Z is at the 4-position.~~

~~45. The compound of any one of claims 1-31 and 33-41, wherein one Z is at the 3-position and the other Z is at the 4-position.~~

~~46. The compound of any one of claims 1-45, wherein Q is a bond.~~

~~47~~13. The compound of any one of claims 1-45, wherein Q is NH, O, S, Q', NH-Q', N(C_1-C_3 alkyl)-Q', O-Q', S-Q', S(O)-Q', or S($O)_2$-Q'.

~~48. The compound of any one of claims 1-45, wherein Q is NH, O, S, or Q'.~~

~~49. The compound of any one of claims 1-45, wherein Q is Q', NH-Q', O-Q', or S-Q'.~~

~~50~~14. The compound of any one of claims 1-12~~45 and 47-49,~~ wherein Q' is a carbon linker comprising one or more $C(R_Q)_2$-$C(R_Q)_2$, ~~or~~ $C(R_Q)_2$ and ~~.~~

~~51. The compound of any one of claims 1-45 and 47-49, wherein Q' is a carbon linker comprising one or more~~ CR_Q=CR_Q.

~~52. The compound of any one of claims 1-45 and 47-49, wherein Q' is a carbon linker comprising one or more C≡C.~~

~~53. The compound of any one of claims 1-45 and 47-49, wherein Q' is a carbon linker comprising one or more $C(R_Q)_2$-$C(R_Q)_2$, $C(R_Q)_2$, and CR_Q=CR_Q.~~

~~54. The compound of any one of claims 1-45 and 47-49, wherein Q' is a carbon linker comprising one or more $C(R_Q)_2$-$C(R_Q)_2$, $C(R_Q)_2$, and C≡C.~~

~~55. The compound of any one of claims 1-45 and 47-49, wherein Q' is a carbon linker comprising one or more CR_Q=CR_Q and C≡C.~~

~~56~~15. The compound of any one of claims 1-~~55~~13, wherein T is cyclopropyl, cyclobutyl, cyclobutenyl, cyclopentyl, cyclopentenyl, cyclohexyl, cyclohexenyl, cycloheptyl, cycloheptenyl, ~~or~~ cyclooctyl or cyclooctenyl, each of which is optionally substituted with one or more R_T or ~~.~~

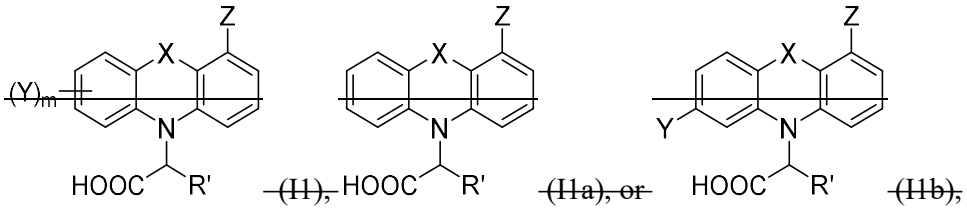
~~57. The compound of any one of claims 1-55, wherein T is cyclobutenyl, cyclopentenyl, cyclohexenyl, cycloheptenyl, or cyclooctenyl, each of which is optionally substituted with one or more R_T.~~

~~58. The compound of any one of claims 1-55,~~ wherein T is heterocyclyl comprising one or two 5- or 6-membered rings and 1-4 heteroatoms selected from N, O, and S, optionally substituted with one or more R_T or ~~.~~

~~59. The compound of any one of claims 1-55, wherein T is C_6-C_{10} aryl optionally substituted with one or more R_T.~~

~~60. The compound of any one of claims 1-55,~~ wherein T is heteroaryl comprising one or two 5- or 6-membered rings and 1-4 heteroatoms selected from N, O, and S, optionally substituted with one or more R_T.

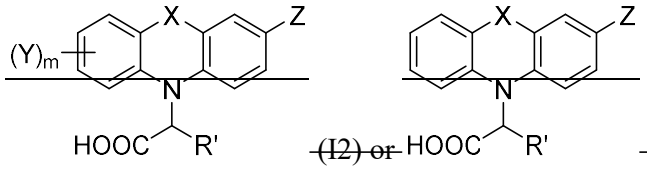
~~61. The compound of claim 1, of Formula I1, I1a, or I1b:~~



~~(I1), (I1a), or (I1b),~~

~~or a pharmaceutically acceptable salt or ester thereof, wherein R' is H or methyl.~~

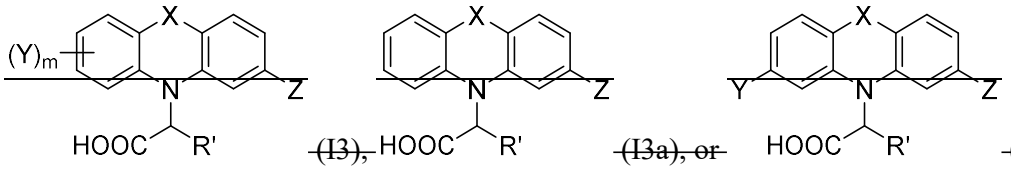
~~62. The compound of claim 1, of Formula I2 or I2a:~~



~~(I2) or (I2a),~~

~~or a pharmaceutically acceptable salt or ester thereof, wherein R' is H or methyl.~~

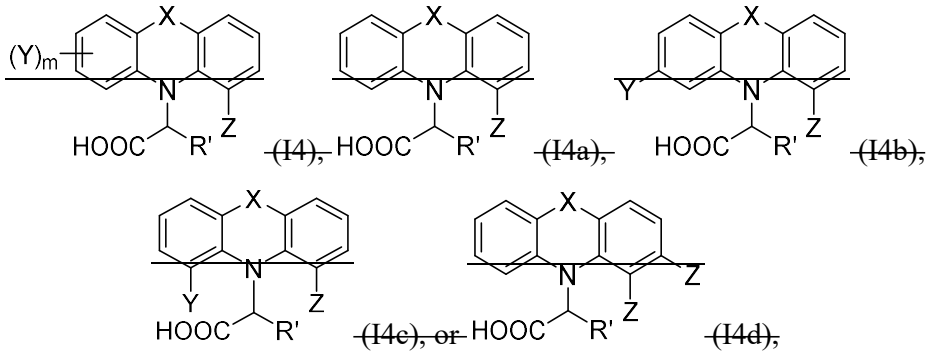
~~63. The compound of claim 1, of Formula I3, I3a, or I3b:~~



~~(I3), (I3a), or (I3b),~~

~~or a pharmaceutically acceptable salt or ester thereof, wherein R' is H or methyl.~~

~~64. The compound of claim 1, of Formula I4, I4a, I4b, I4c, or I4d:~~

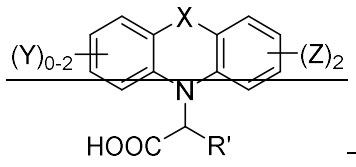


~~(I4), (I4a), (I4b),~~

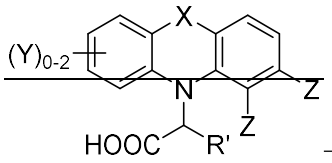
~~(I4c), or (I4d),~~

~~or a pharmaceutically acceptable salt or ester thereof, wherein R' is H or methyl.~~

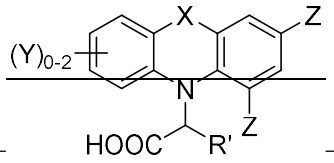
~~65. The compound of claim 1, of Formula I5, I5a1, I5a2, I5a3, I5a4, I5a5, I5a6, I5b1, I5b2, I5b3, I5b4, I5b5, I5b6, I5c1, I5c2, I5c3, I5c4, I5c5, I5c6, I5d1, I5d2, I5d3, I5d4, I5d5, or I5d6:~~



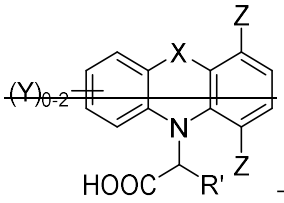
~~(I5),~~



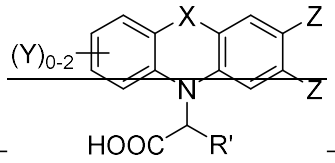
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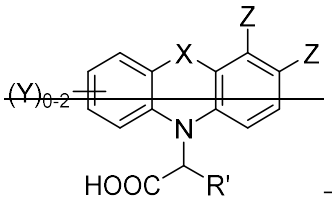
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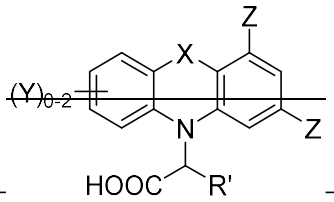
~~(I5a3),~~



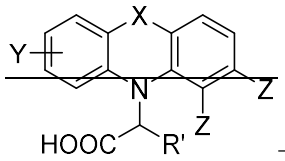
~~(I5a4),~~



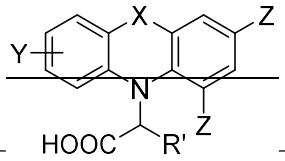
~~(I5a5),~~



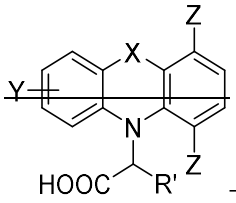
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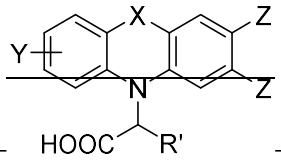
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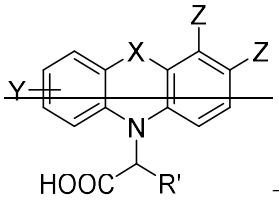
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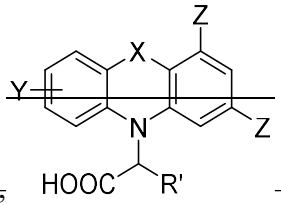
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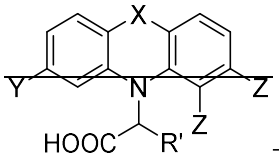
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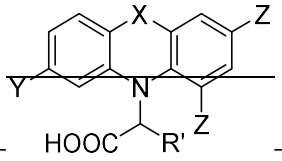
~~(I5b5),~~



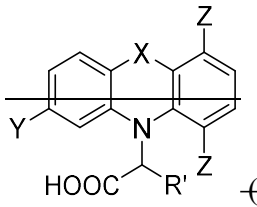
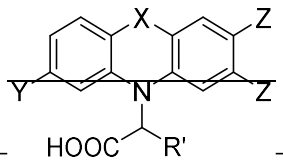
~~(I5b6),~~

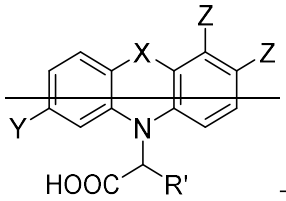
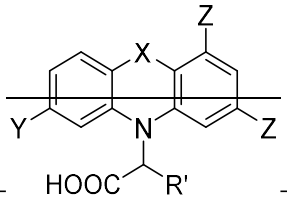


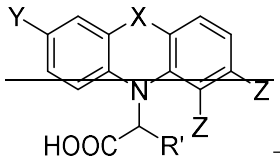
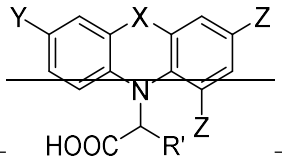
~~(I5c1),~~

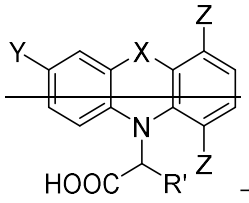
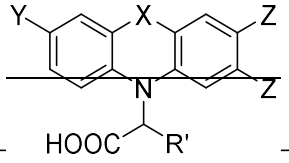


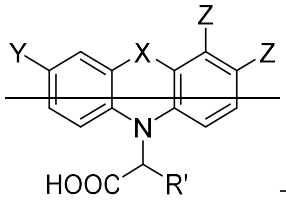
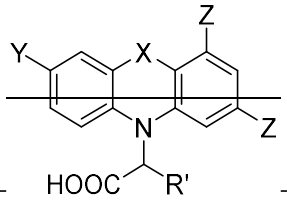
~~(I5c2),~~


~~(I5c3),~~ 
~~(I5c4),~~


~~(I5c5),~~ 
~~(Ic56),~~

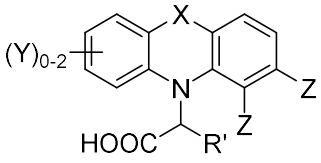
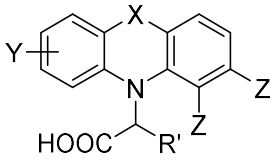

~~(I5d1),~~ 
~~(I5d2),~~

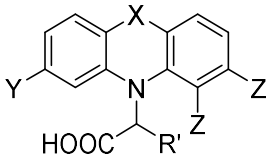
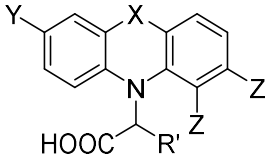

~~(I5d3),~~ 
~~(I5d4),~~


~~(I5d5), or~~ 
~~(I5d6),~~

~~or a pharmaceutically acceptable salt or ester thereof, wherein R' is H or methyl.~~

~~66~~16. The compound of claim 1, of Formula I5a1, I5b1, I5c1, or I5d1:


(I5a1), 
(I5b1),


(I5c1), or 
(I5d1),

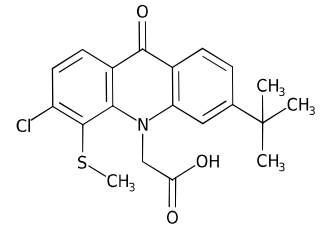
or a pharmaceutically acceptable salt or ester thereof, wherein R' is H or methyl.

~~67. The compound of claim 1, selected from Table 1.~~

~~68~~17. The compound of claim ~~67~~1, wherein R' is H, Y is *tert*-butyl at the 6-position, one Z is Cl at the 3-position, and the other Z is S-CH_3 at the 4-position or~~.~~

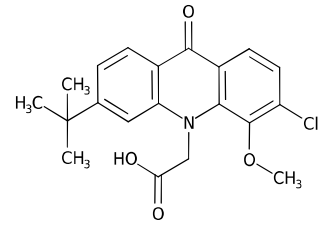
~~69. The compound of claim 67, wherein R' is H, Y is *tert* butyl at the 6-position, one Z is Cl at the 3-position, and the other Z is~~ O-CH_3 at the 4-position.

18. The compound of claim 1, wherein the compound is:



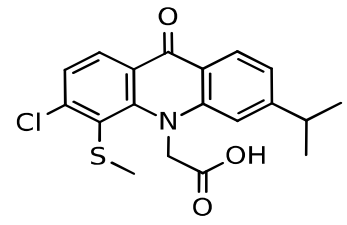
or a pharmaceutically acceptable salt of ester thereof.

19. The compound of claim 1, wherein the compound is:



or a pharmaceutically acceptable salt of ester thereof.

20. The compound of claim 1, wherein the compound is:



or a pharmaceutically acceptable salt or ester thereof.

~~70~~21. A pharmaceutical composition comprising a therapeutically effective amount of a compound of any one of claims 1-~~69~~20, or a pharmaceutically acceptable salt or ester thereof, and a pharmaceutically acceptable carrier.

~~71. A method of modulating a stimulator of interferon genes (STING) protein, comprising administering to a subject in need thereof an effective amount of a compound of any of claims 1-69 or a pharmaceutically acceptable salt or ester thereof, or the pharmaceutical composition of claim 70.~~

~~72. A method of treating or preventing a disease, wherein the diseases is caused by, or associated with, STING expression, activity, and/or function, or is associated with deregulation of one or more of the intracellular pathways in which a STING protein is involved, comprising administering to a subject in need thereof an effective amount of a compound of any of claims 1-69 or a pharmaceutically acceptable salt or ester thereof, or the pharmaceutical composition of claim 70.~~

~~73. A compound of any of claims 1-69 or a pharmaceutically acceptable salt or ester thereof, or the pharmaceutical composition of claim 70, for use in modulating a STING protein, or in treating or preventing a disease caused by, or associated with, STING expression, activity, and/or function, or associated with deregulation of one or more of the intracellular pathways in which a STING protein is involved.~~

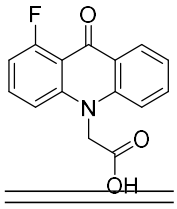
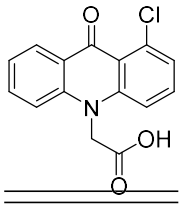
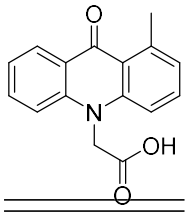
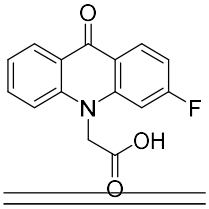
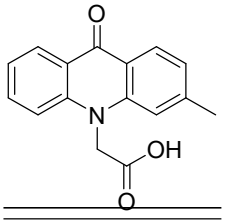
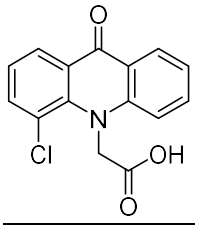
~~74~~22. A compound of any one of claims ~~1-69~~18-20 ~~or a pharmaceutically acceptable salt or ester thereof, or the pharmaceutical composition of claim 70,~~ for use in the manufacture of a medicament for modulating a STING protein, or for treating or preventing a disease caused by, or associated with, STING expression, activity, and/or function, or associated with deregulation of one or more of the intracellular pathways in which a STING protein is involved.

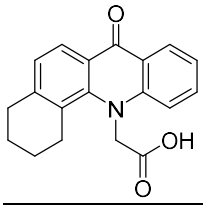
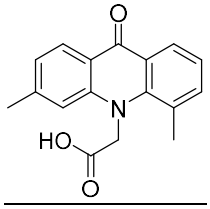
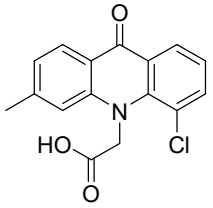
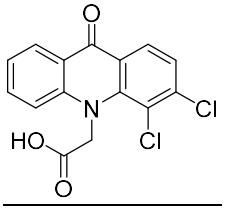
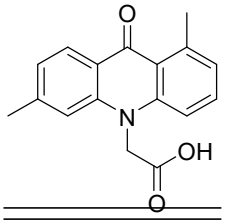
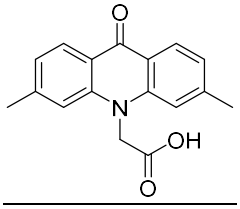
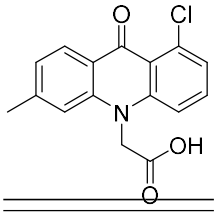
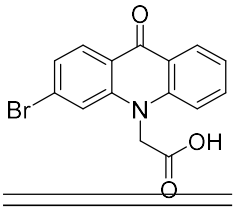
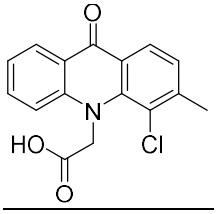
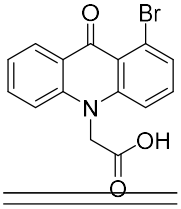
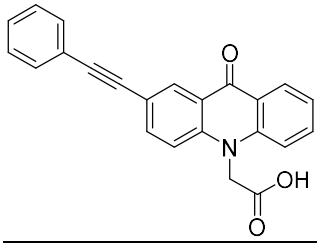
~~75. Use of a compound of any of claims 1-69 or a pharmaceutically acceptable salt or ester thereof, or the pharmaceutical composition of claim 70, in modulating a STING protein, or in treating or preventing a disease caused by, or associated with, STING expression, activity, and/or function, or associated with deregulation of one or more of the intracellular pathways in which a STING protein is involved.~~

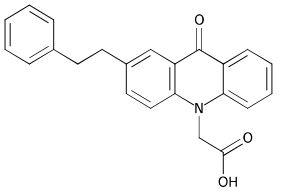
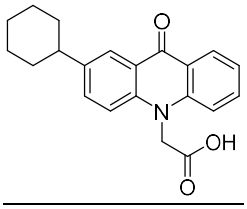
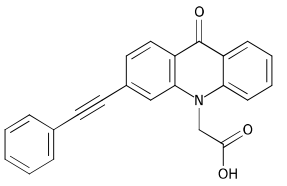
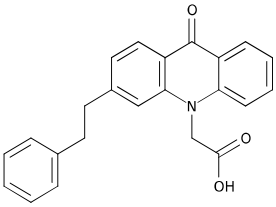
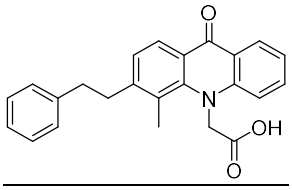
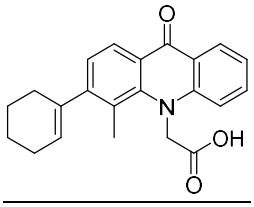
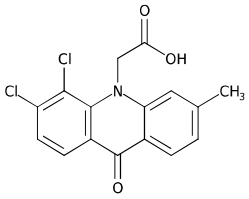
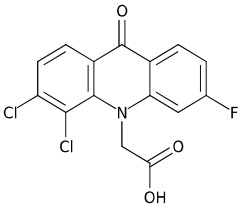
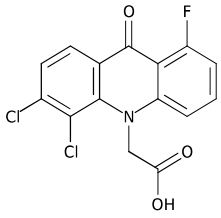
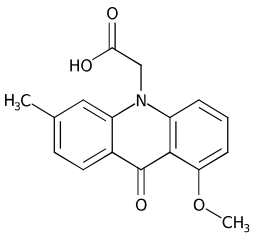
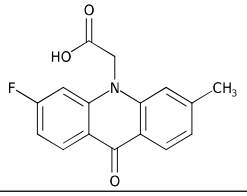
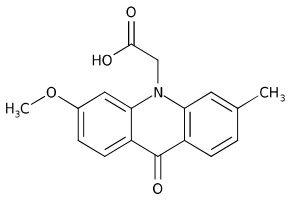
~~76. Use of a compound of any of claims 1-69 or a pharmaceutically acceptable salt or ester thereof, or the pharmaceutical composition of claim 70, in the manufacture of a medicament for modulating a STING protein, or for treating or preventing a disease caused by, or associated with, STING expression, activity, and/or function, or associated with deregulation of one or more of the intracellular pathways in which a STING protein is involved.~~

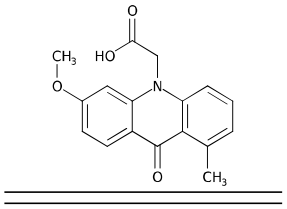
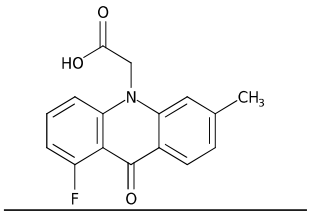
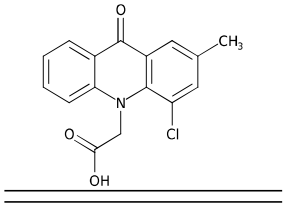
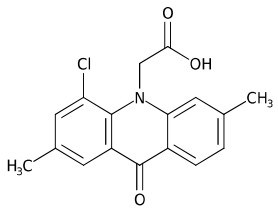
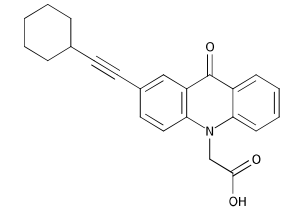
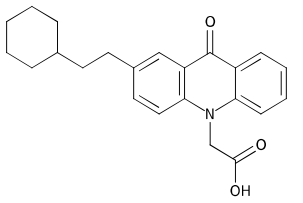
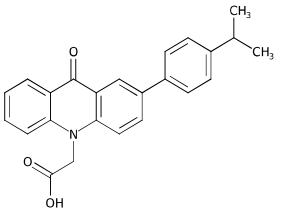
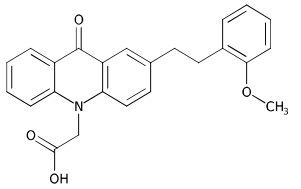
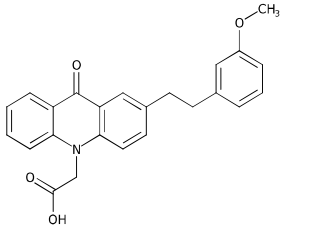
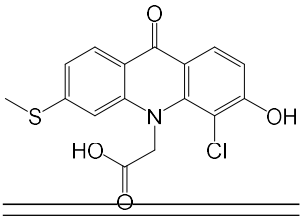
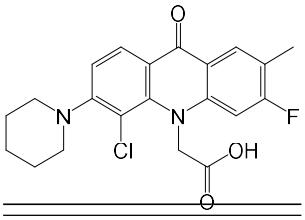
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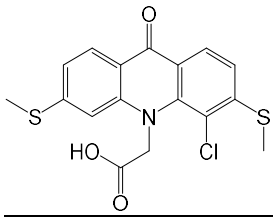
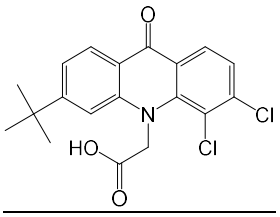
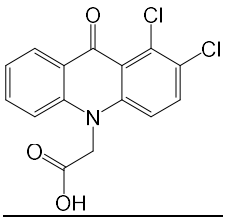
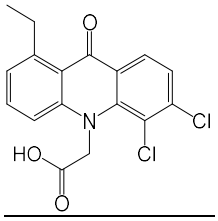
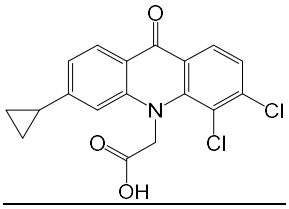
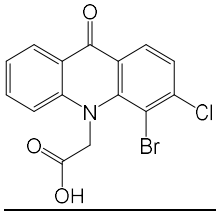
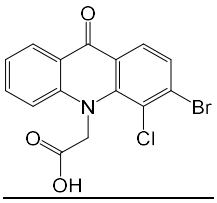
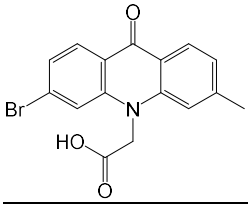
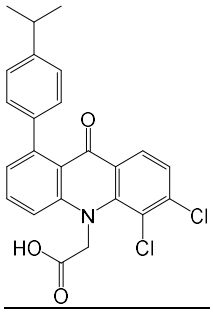
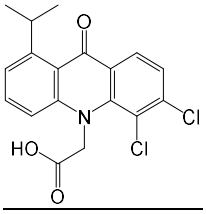
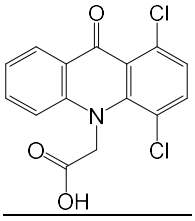
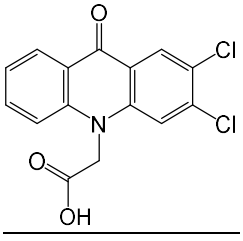
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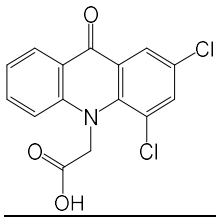
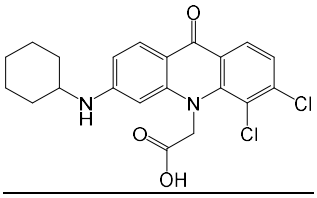
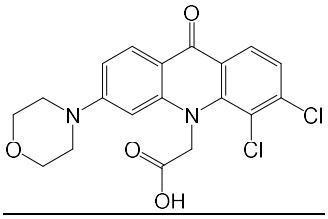
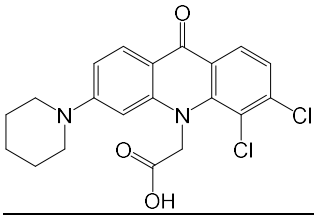
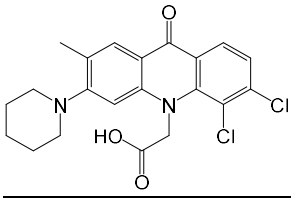
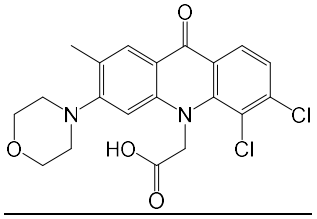
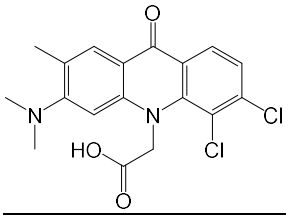
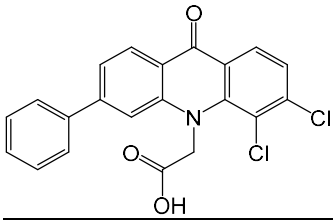
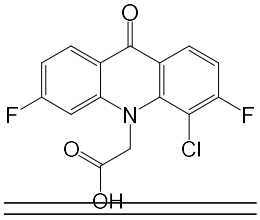
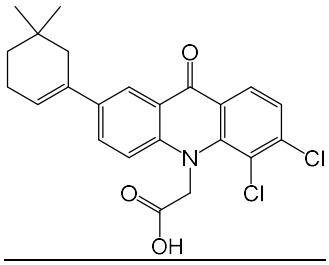
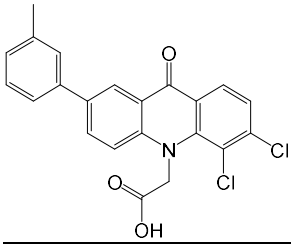
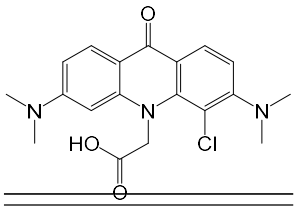
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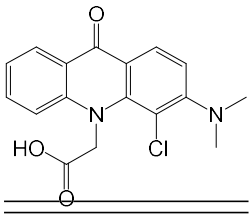
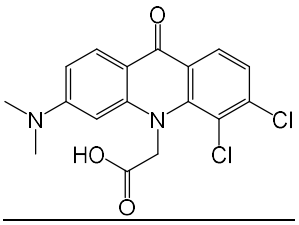
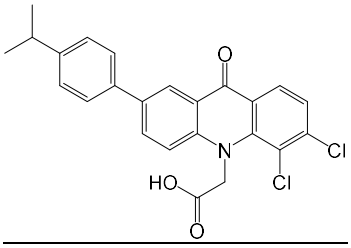
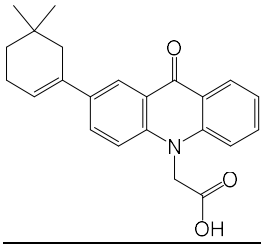
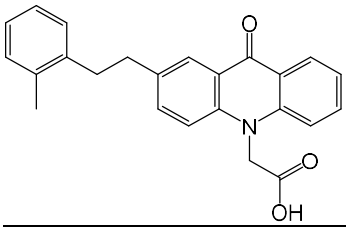
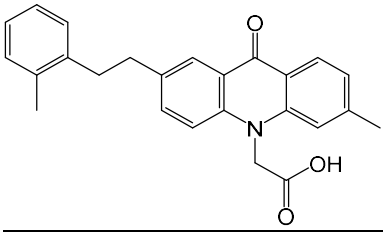
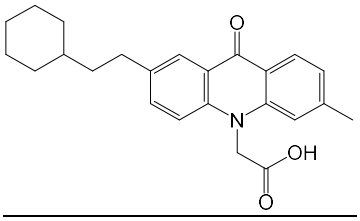
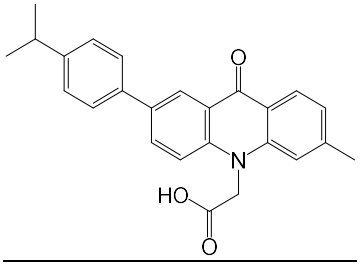
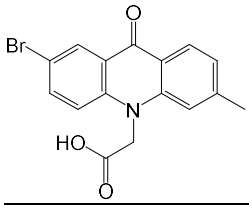
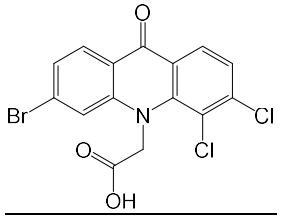
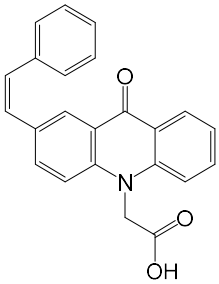
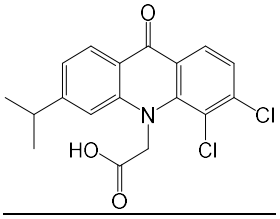
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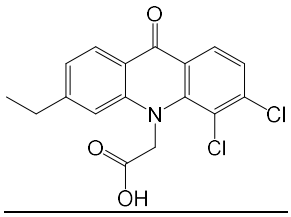
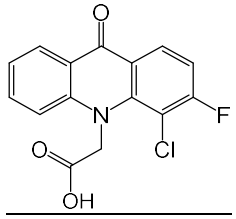
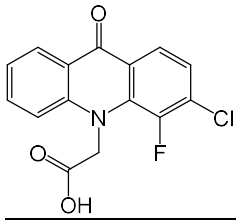
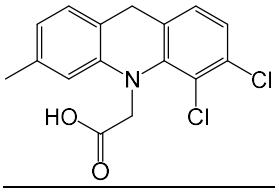
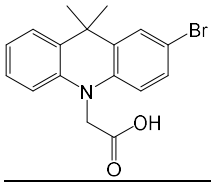
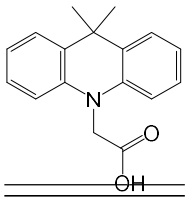
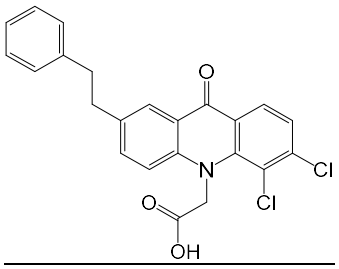
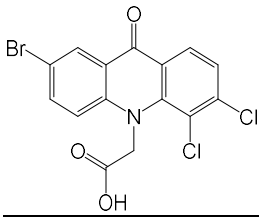
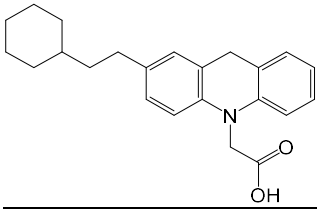
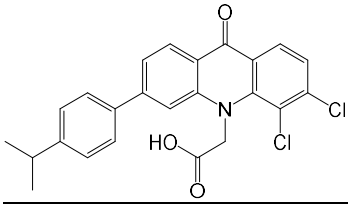
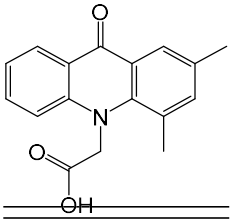
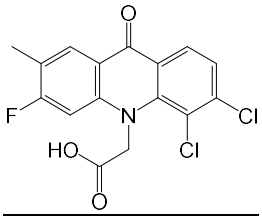
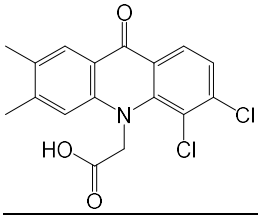
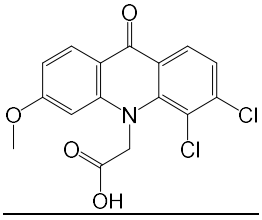
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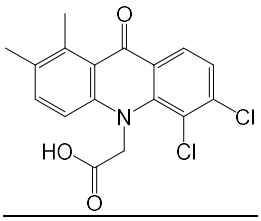
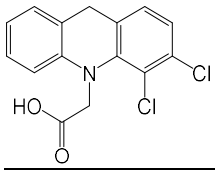
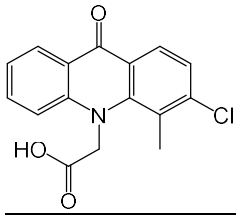
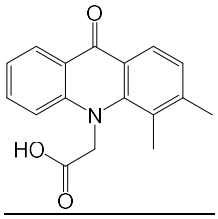
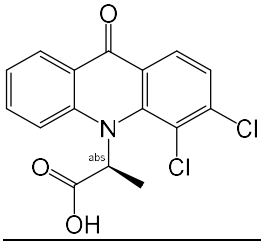
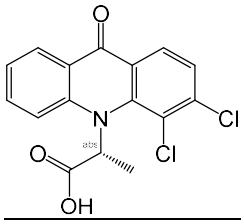
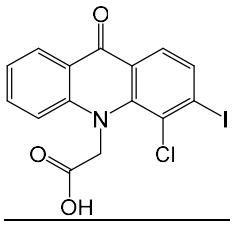
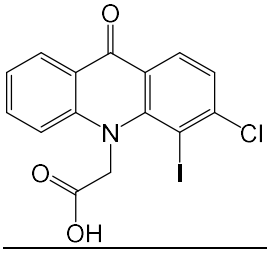
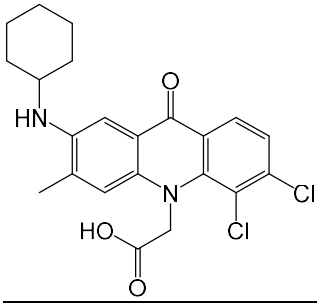
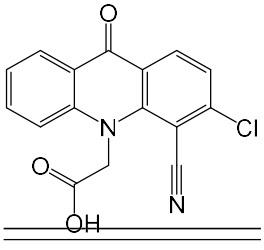
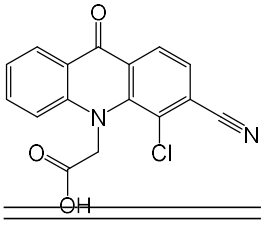
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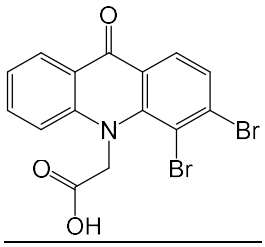
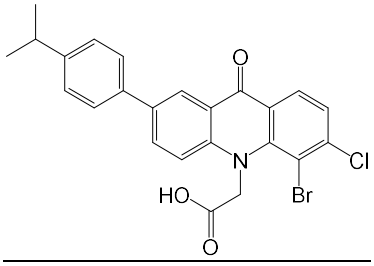
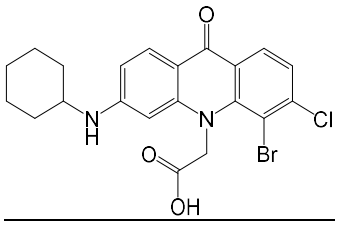
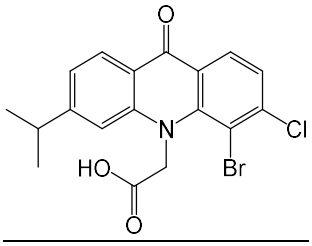
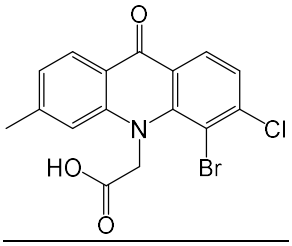
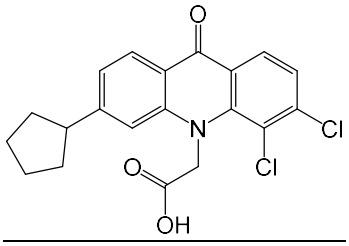
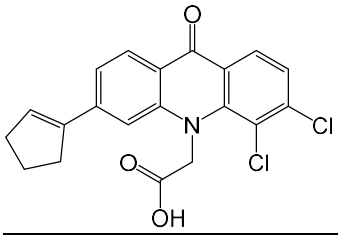
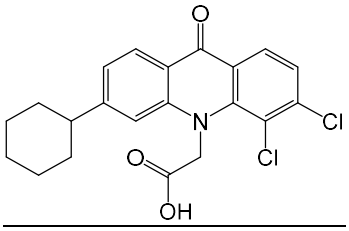
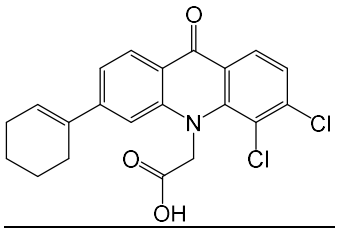
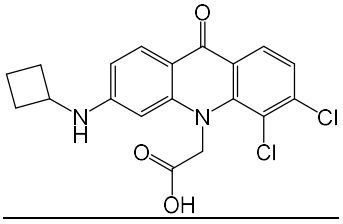
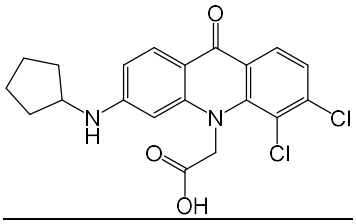
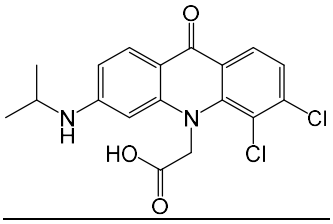
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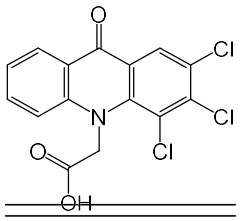
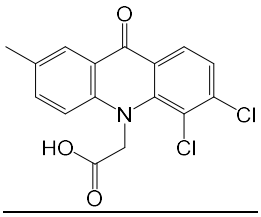
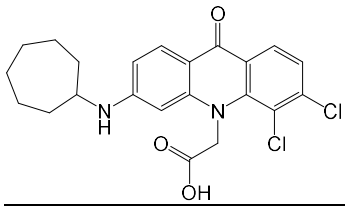
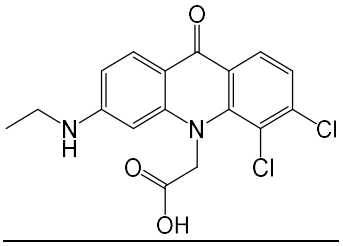
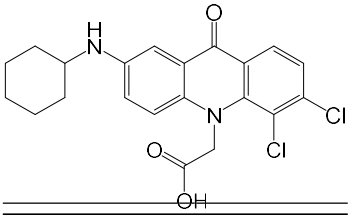
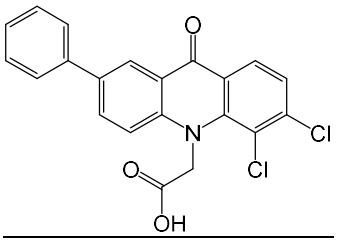
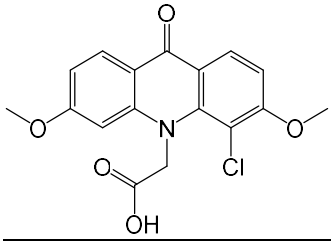
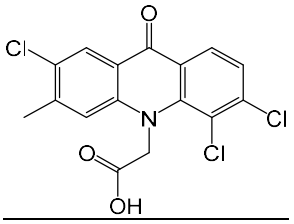
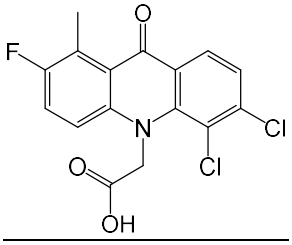
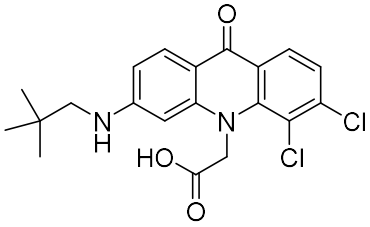
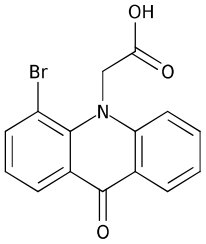
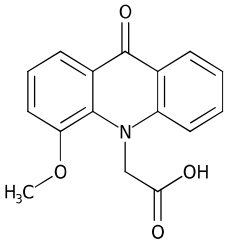
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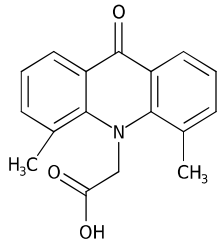
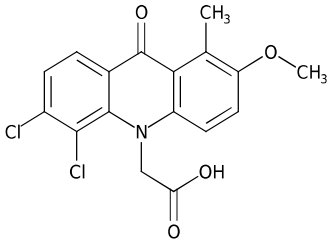
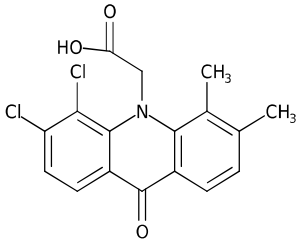
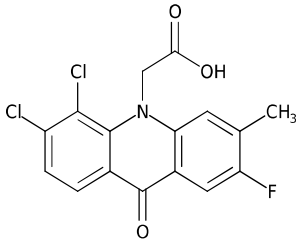
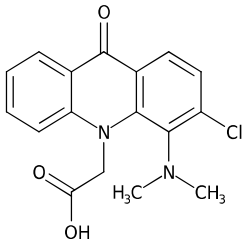
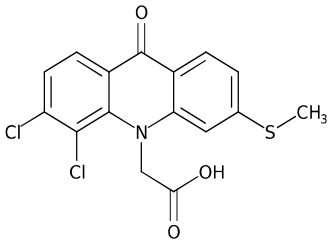
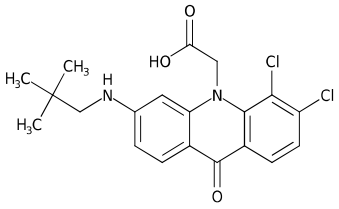
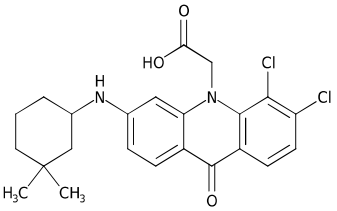
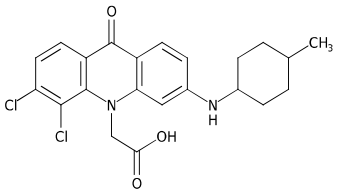
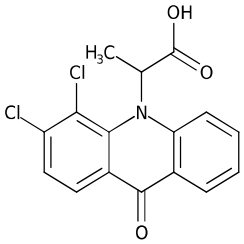
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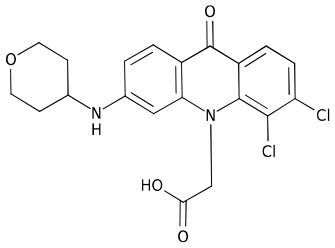
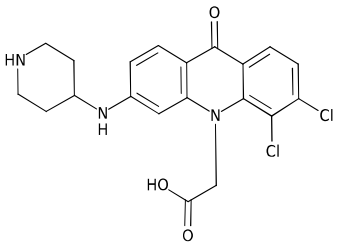
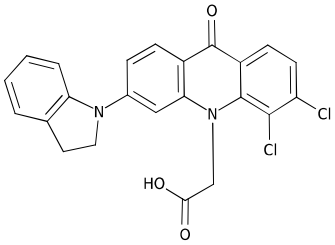
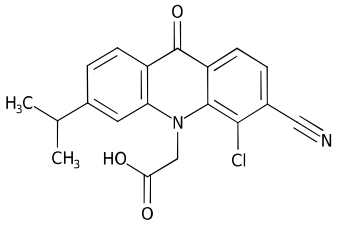
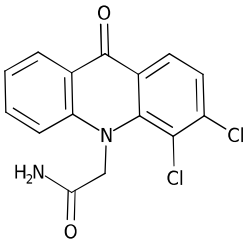
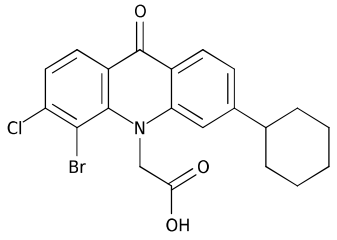
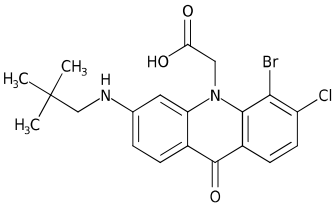
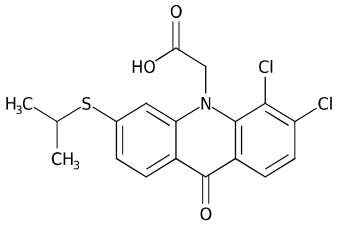
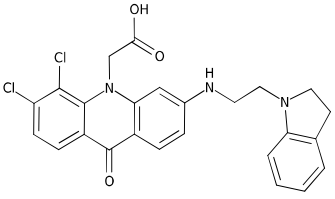
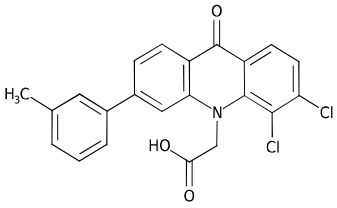
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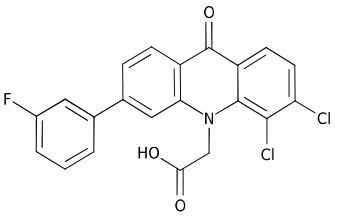
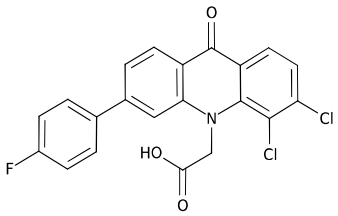
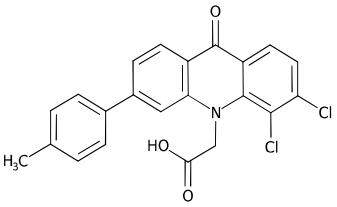
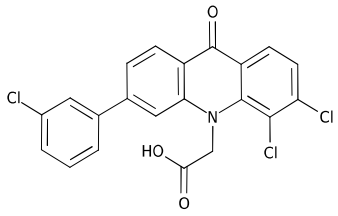
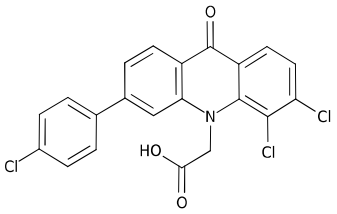
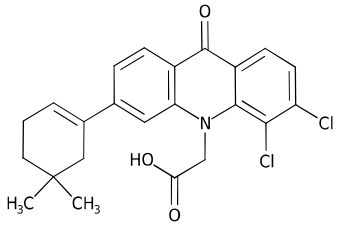
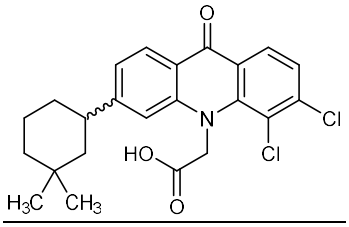
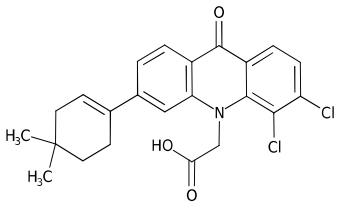
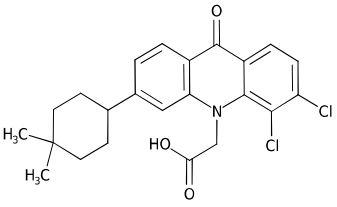
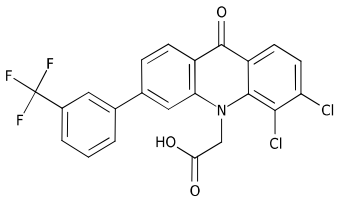
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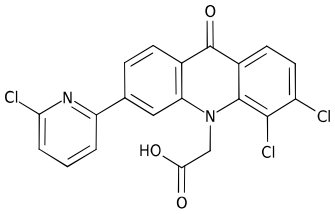
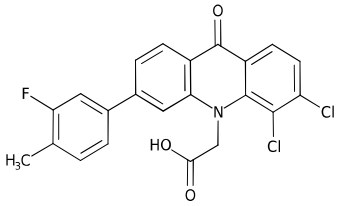
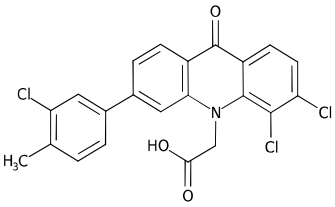
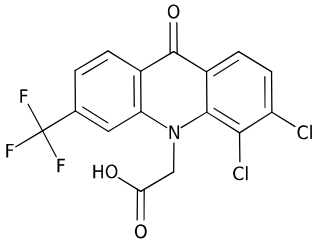
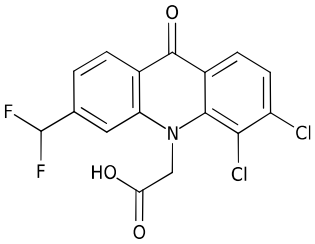
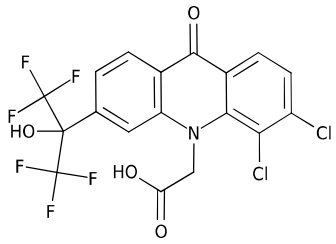
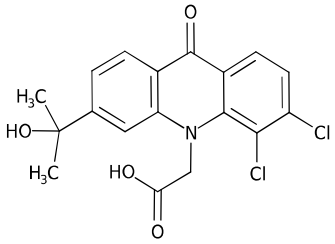
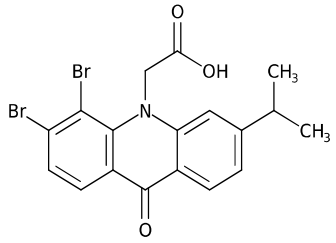
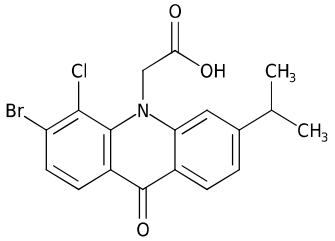
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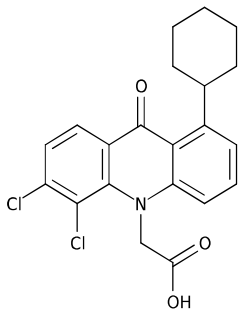
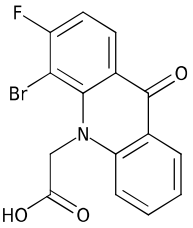
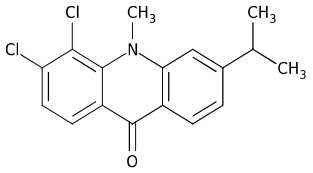
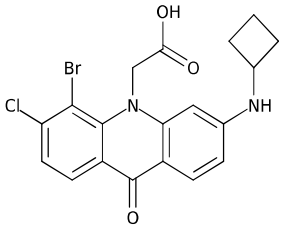
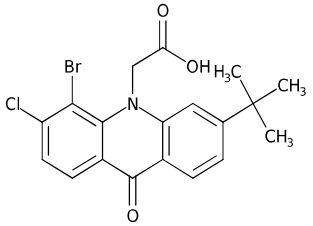
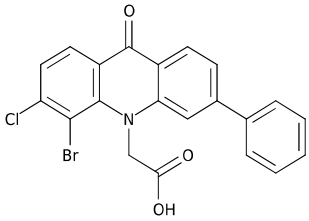
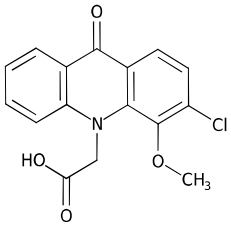
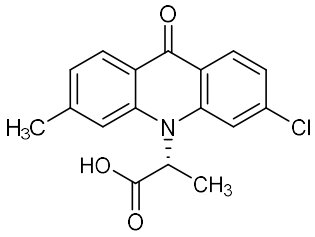
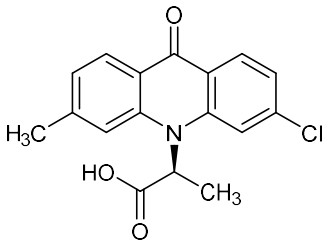
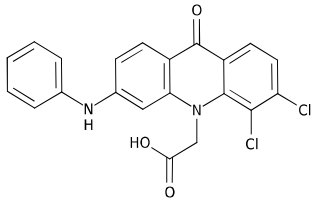
Cmpd No.	Structure	Cmpd No.	Structure
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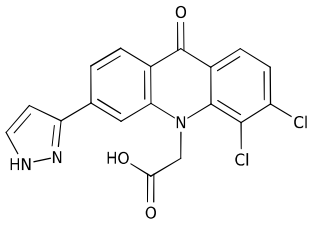
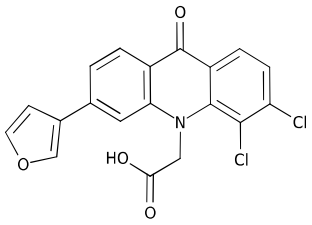
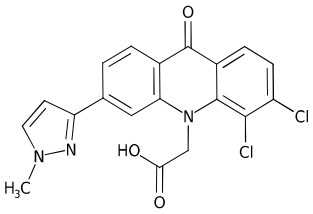
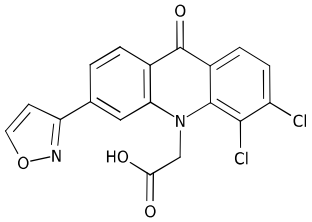
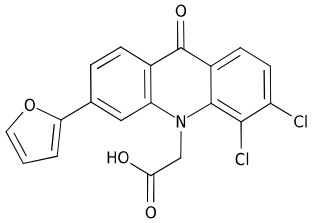
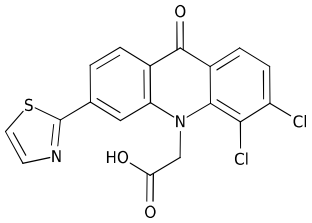
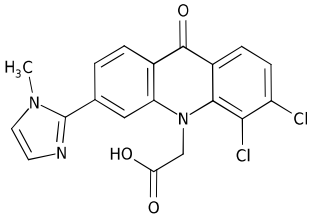
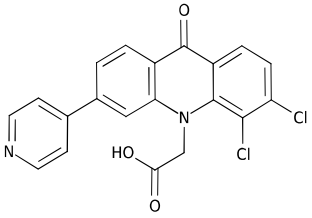
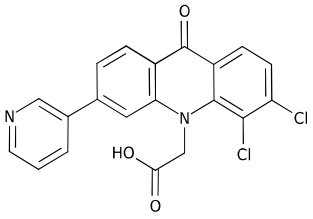
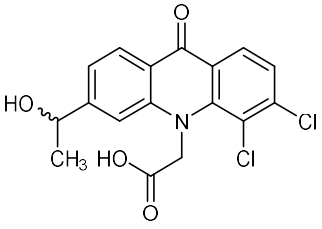
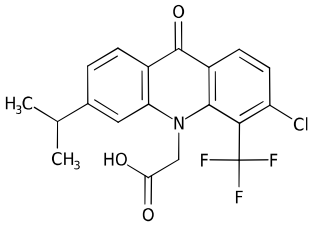
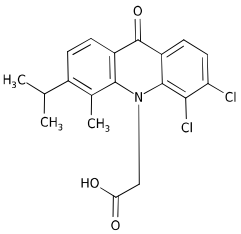
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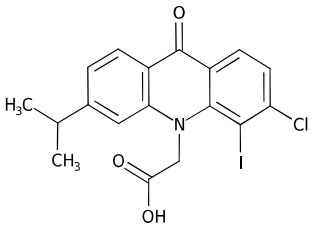
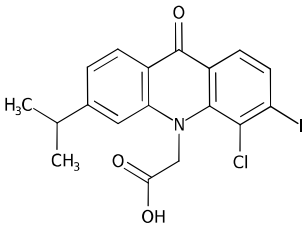
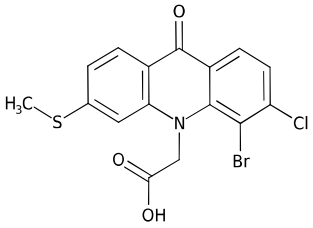
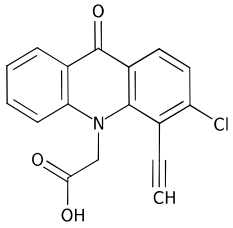
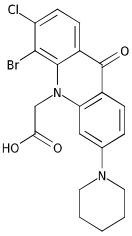
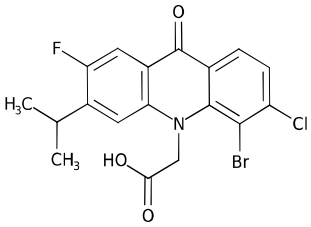
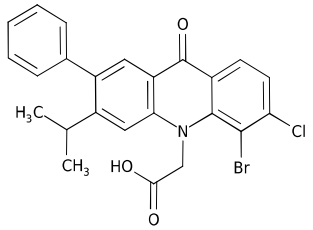
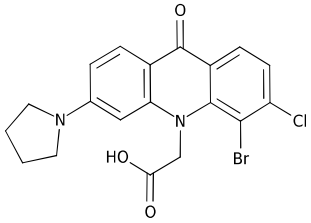
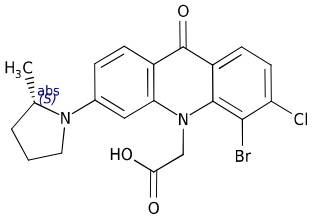
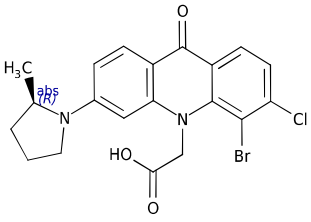
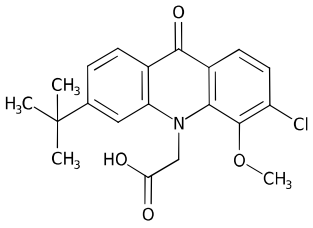
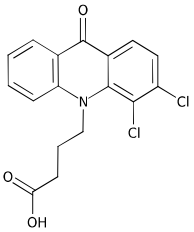
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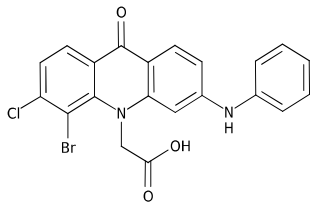
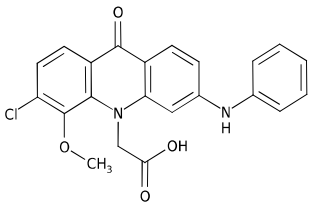
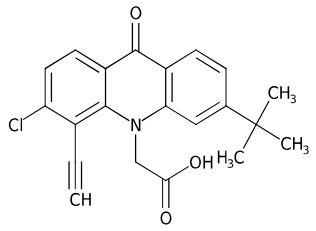
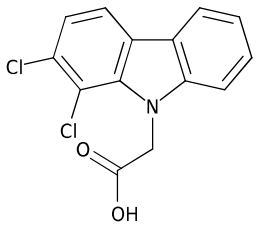
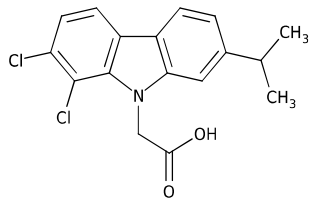
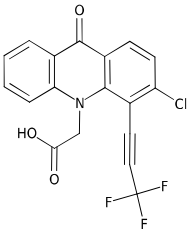
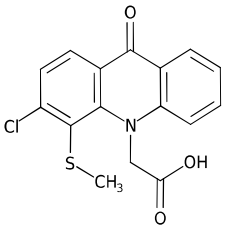
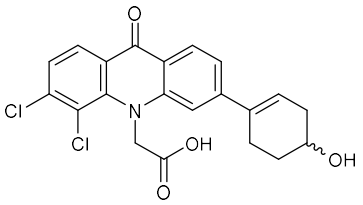
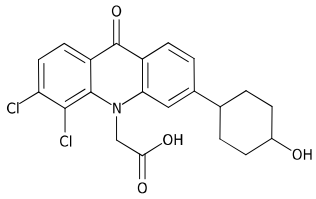
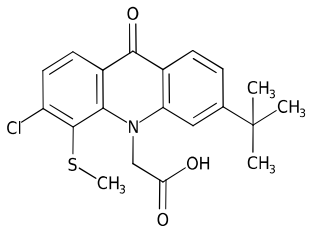
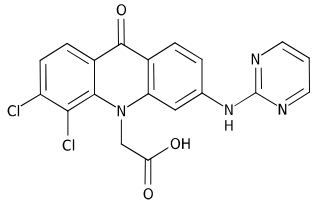
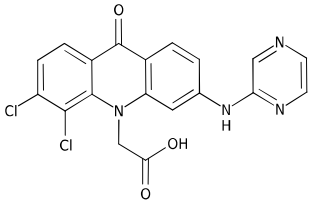
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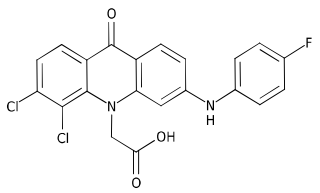
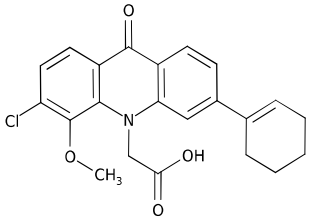
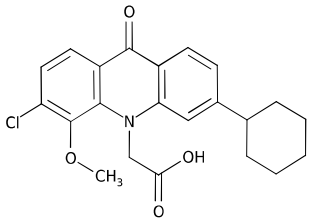
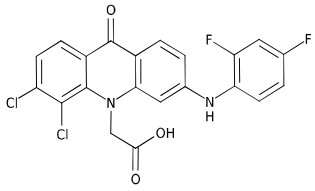
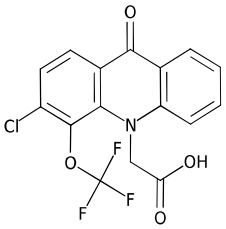
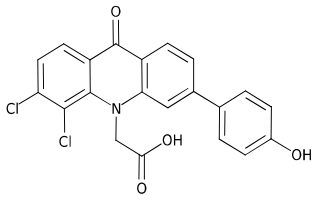
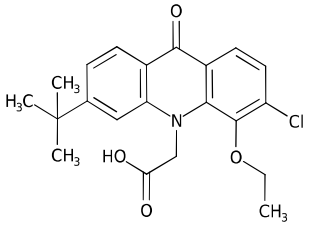
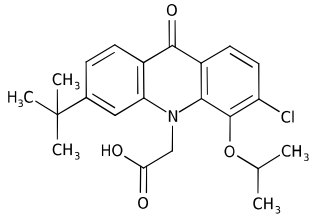
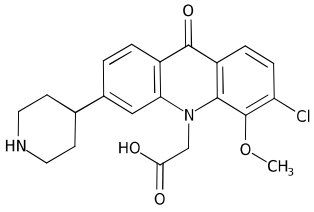
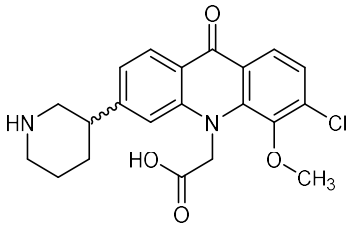
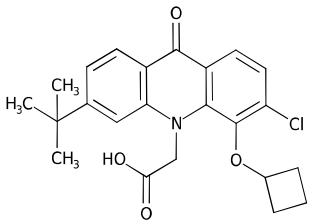
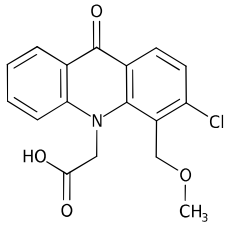
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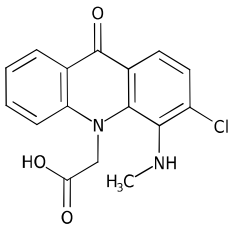
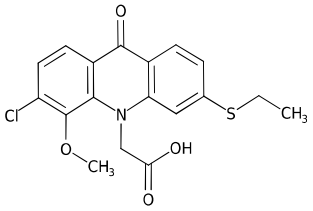
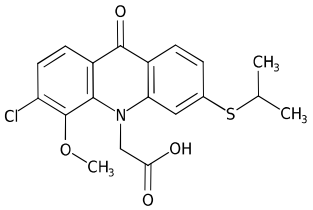
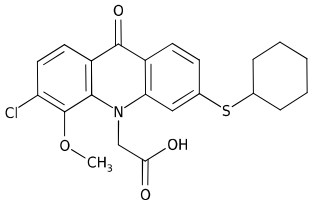
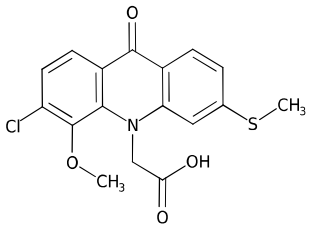
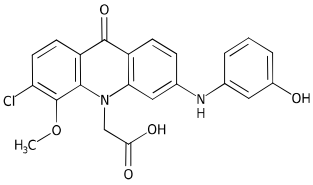
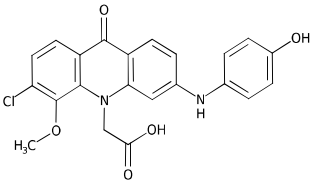
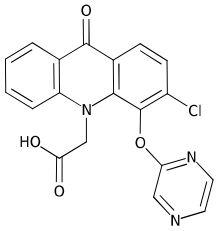
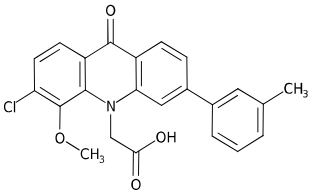
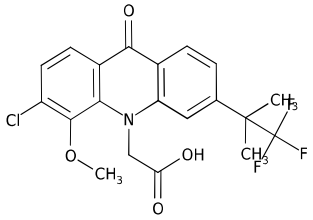
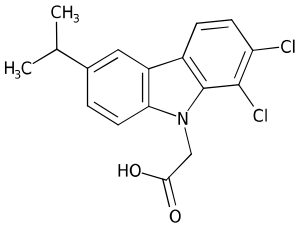
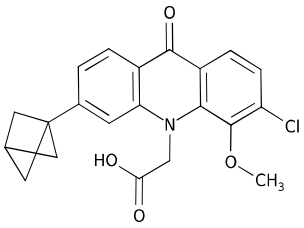
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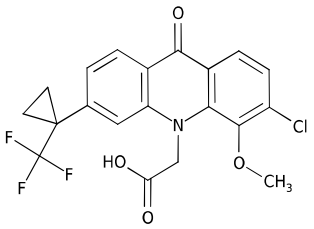
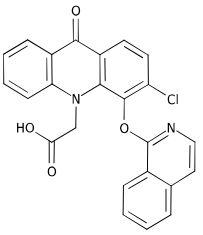
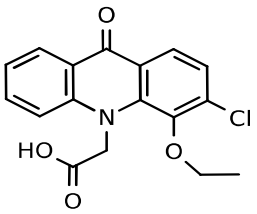
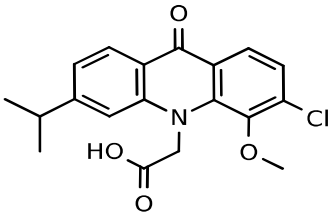
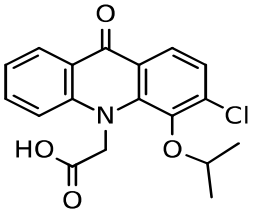
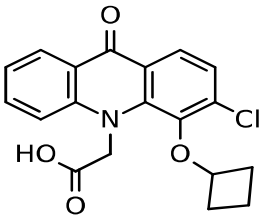
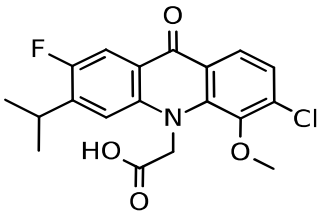
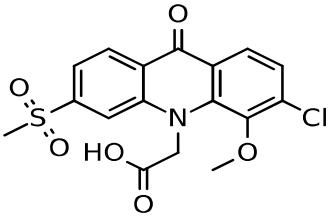
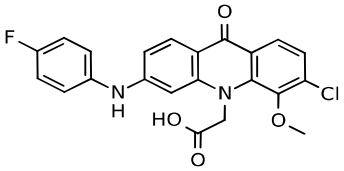
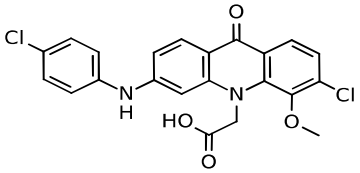
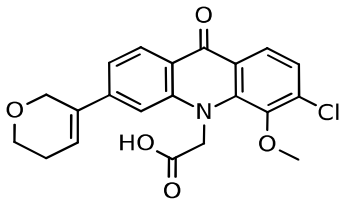
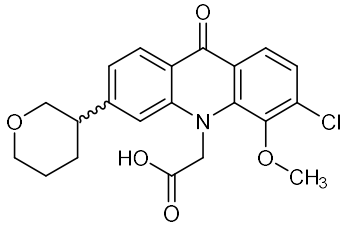
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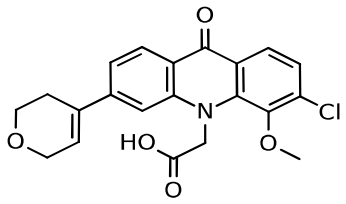
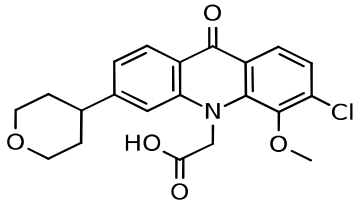
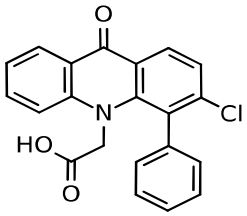
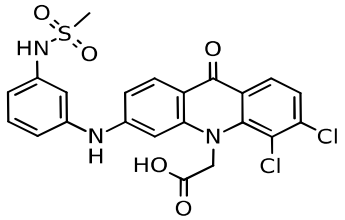
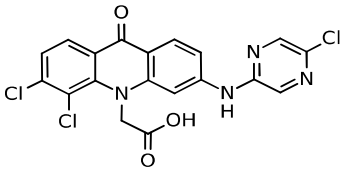
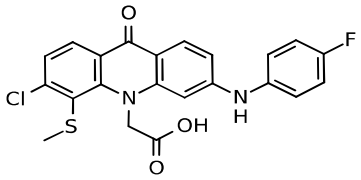
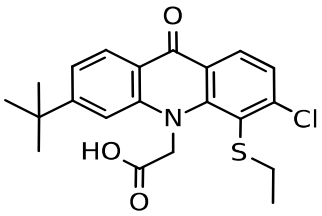
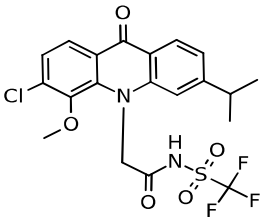
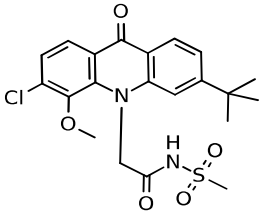
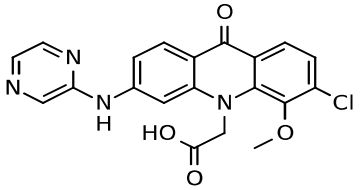
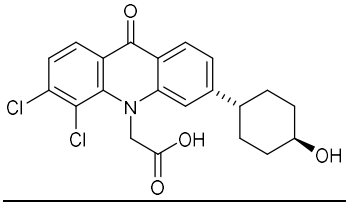
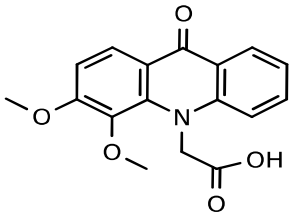
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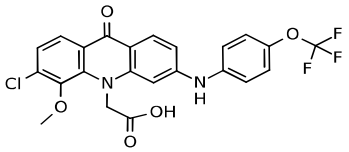
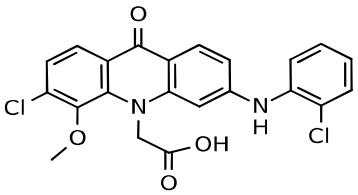
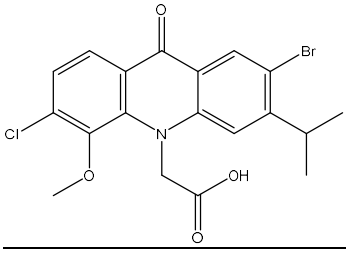
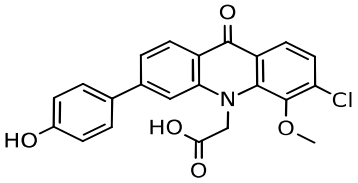
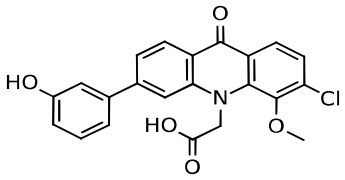
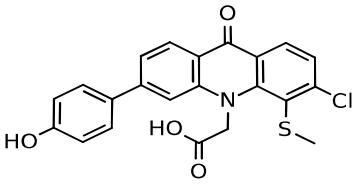
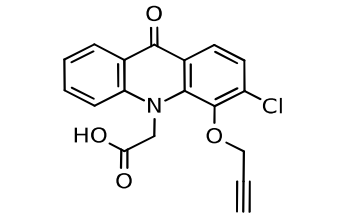
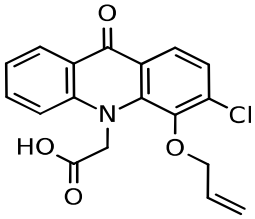
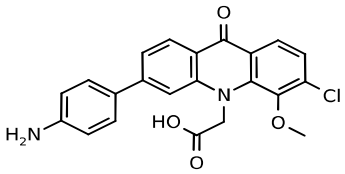
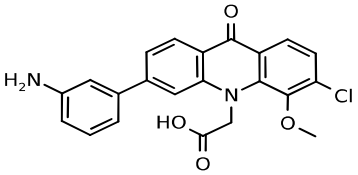
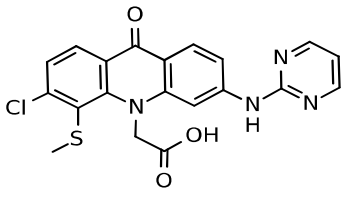
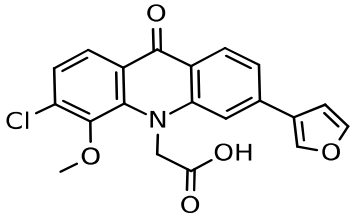
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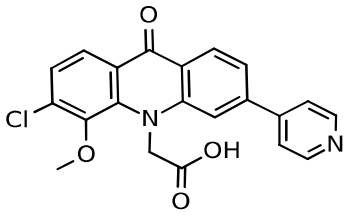
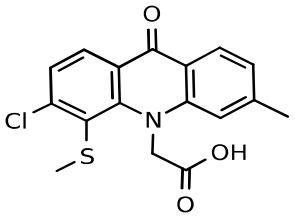
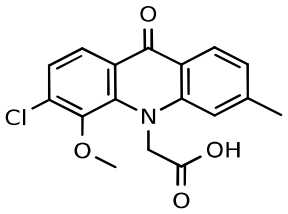
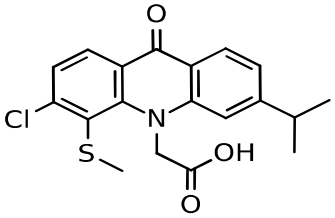
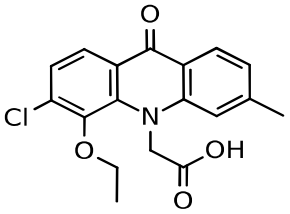
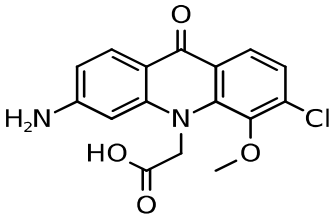
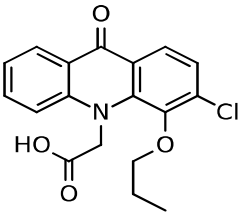
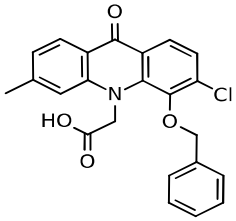
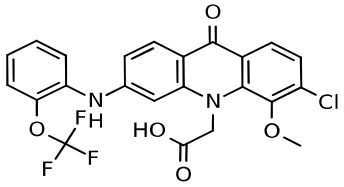
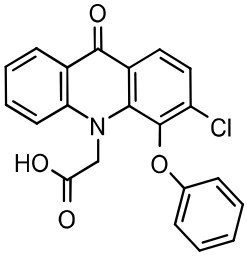
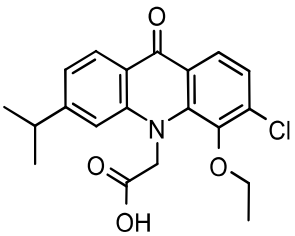
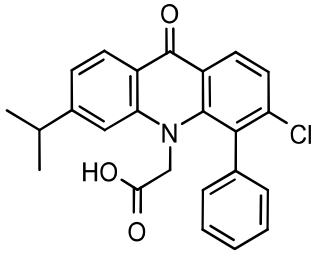
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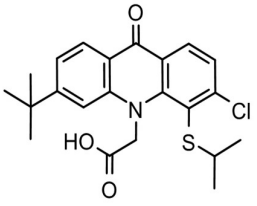
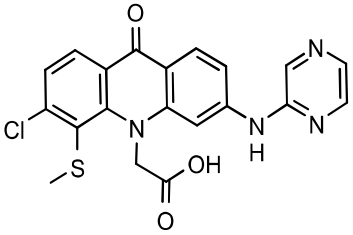
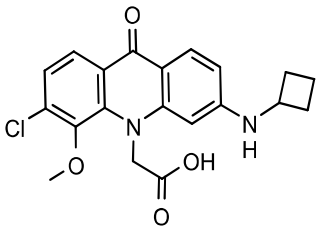
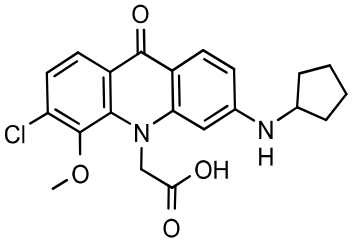
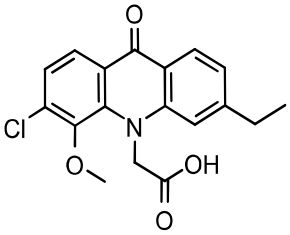
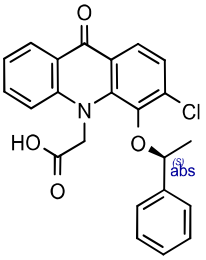
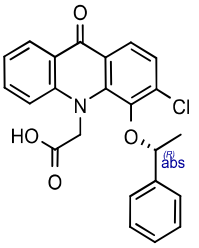
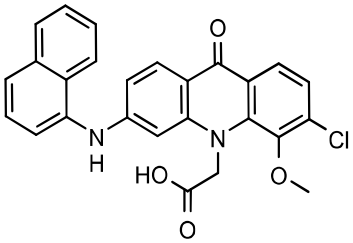
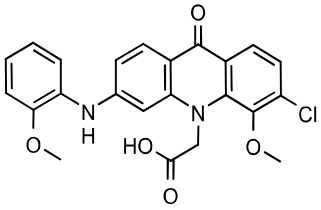
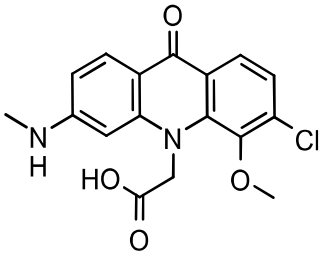
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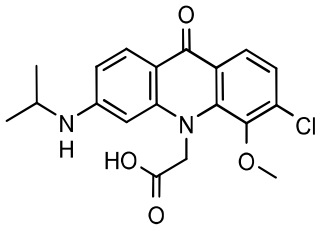
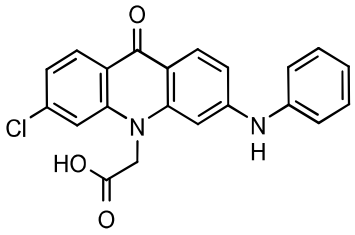
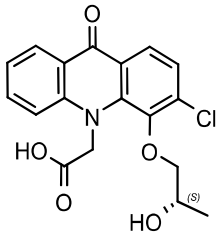
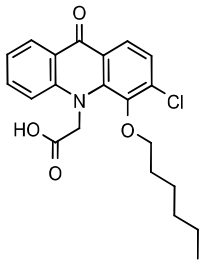
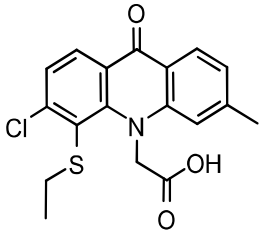
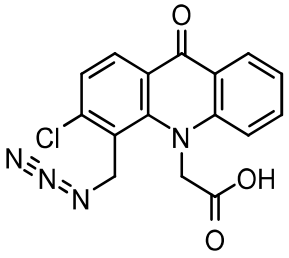
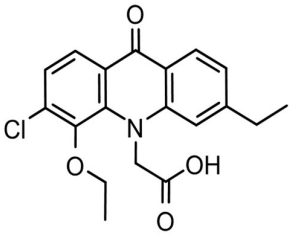
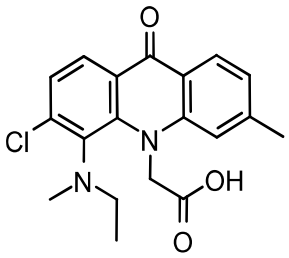
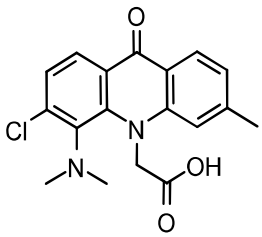
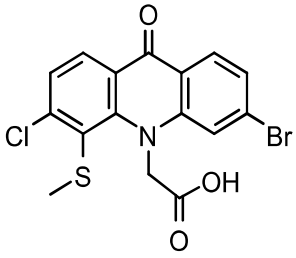
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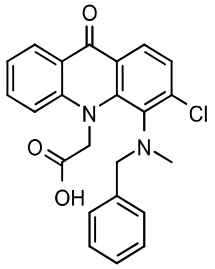
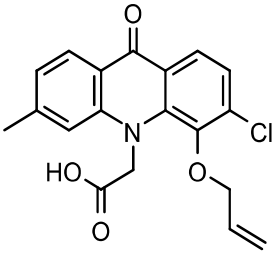
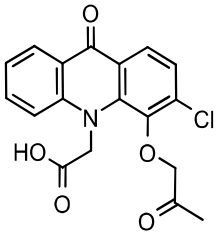
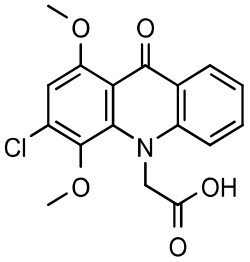
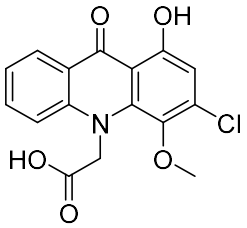
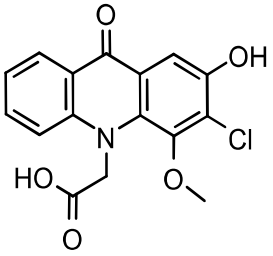
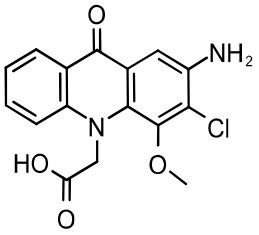
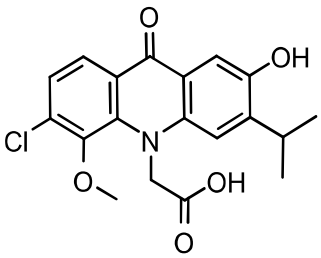
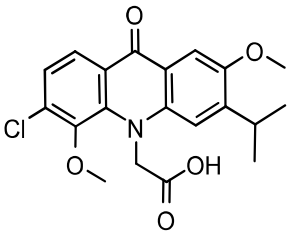
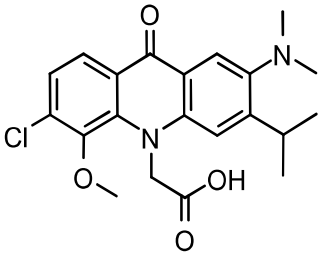
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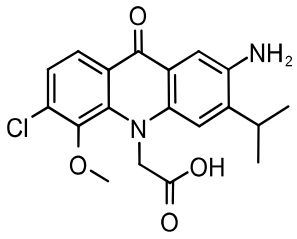
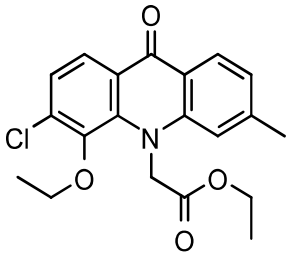
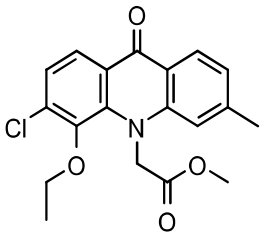
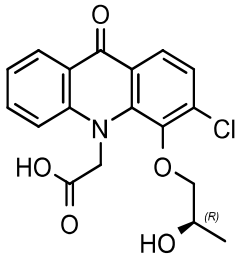
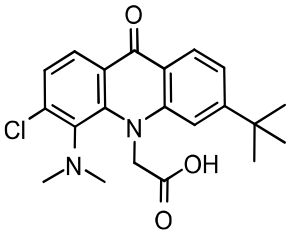
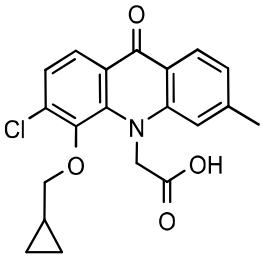
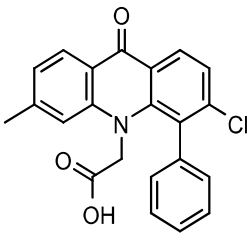
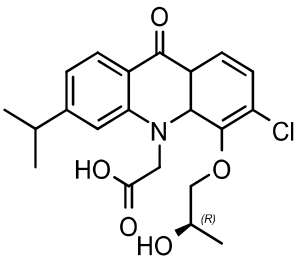
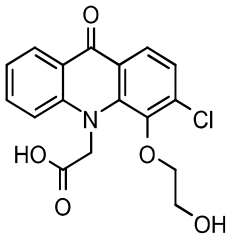
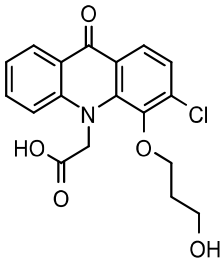
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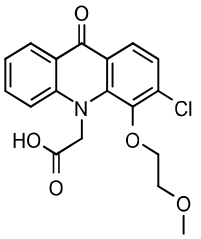
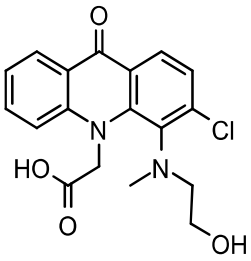
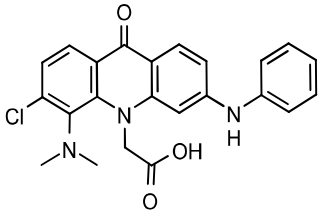
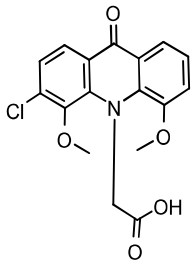
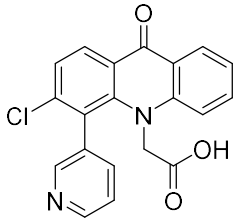
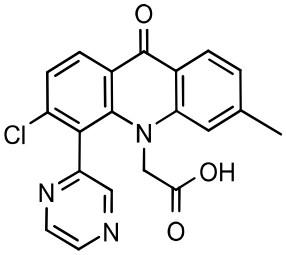
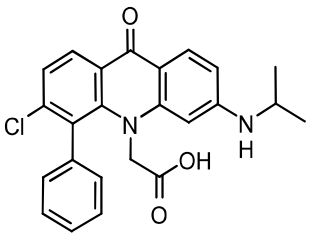
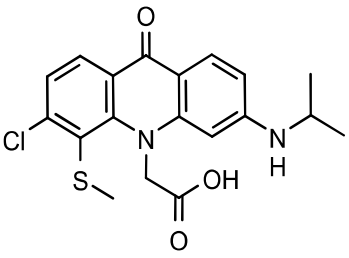
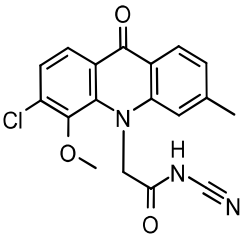
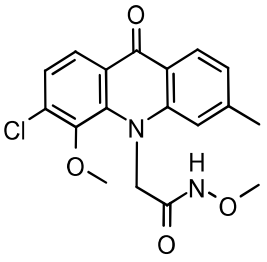
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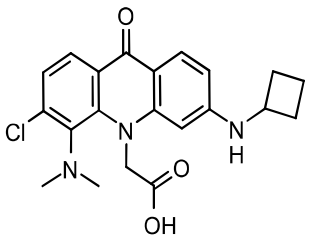
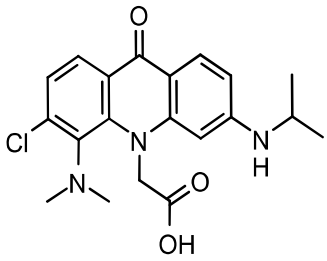
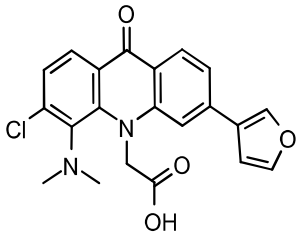
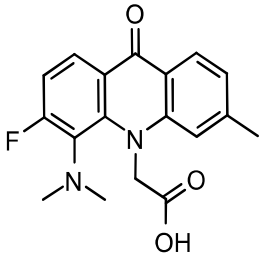
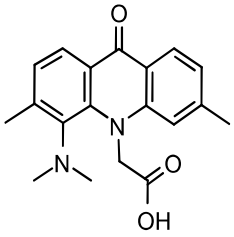
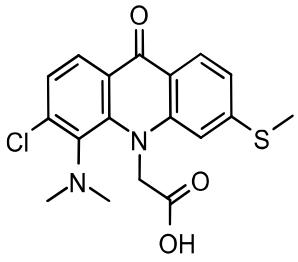
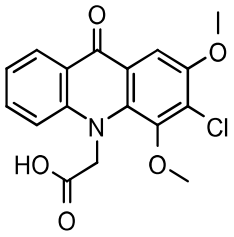
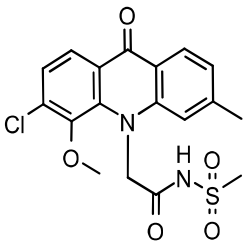
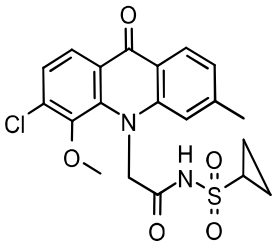
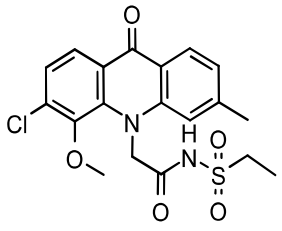
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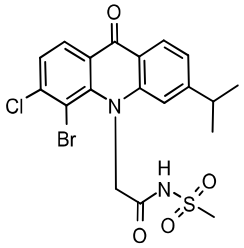
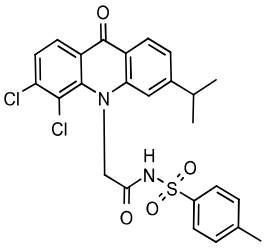
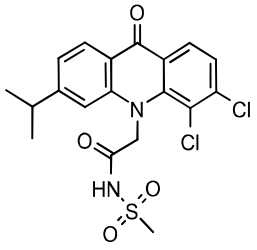
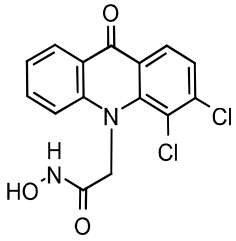
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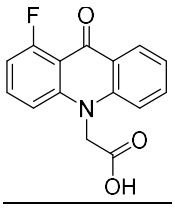
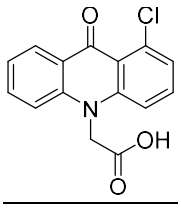
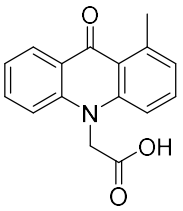
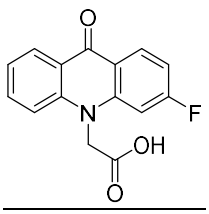
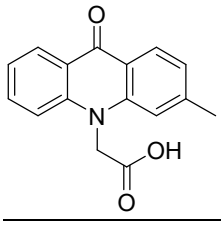
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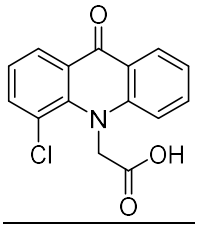
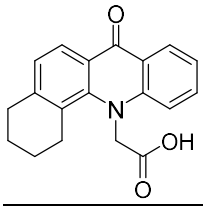
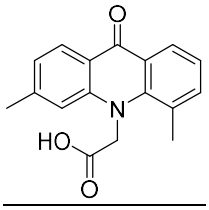
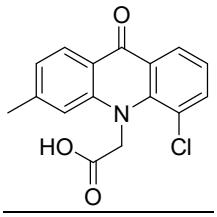
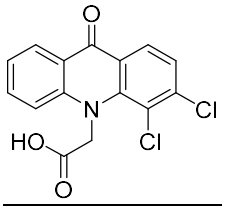
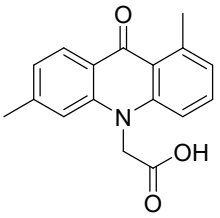
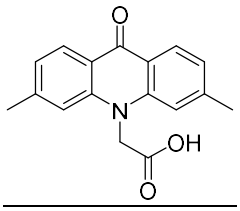
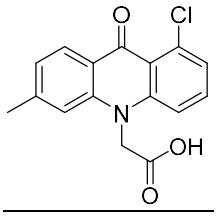
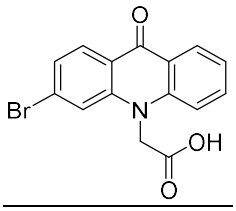
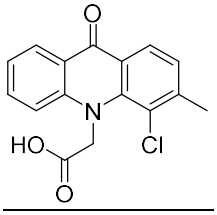
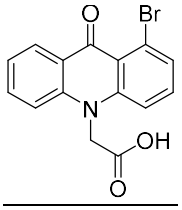
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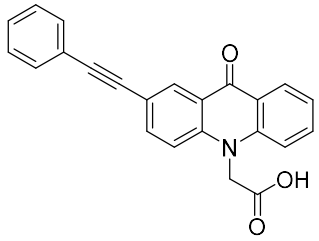
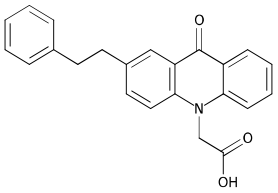
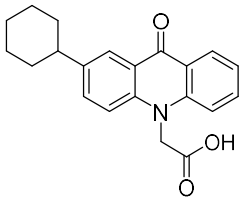
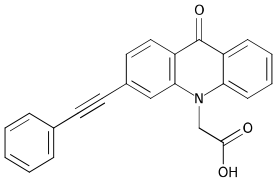
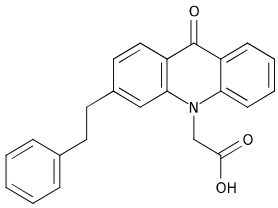
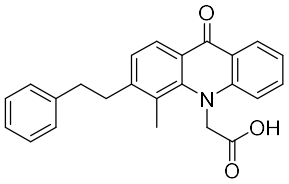
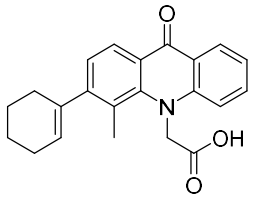
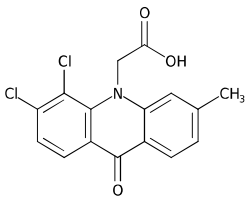
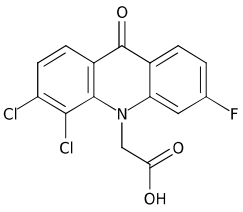
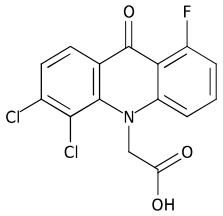
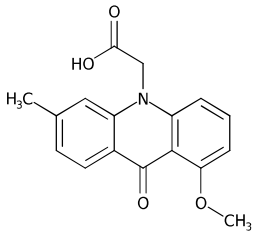
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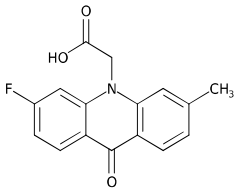
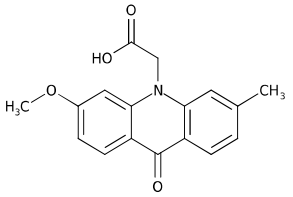
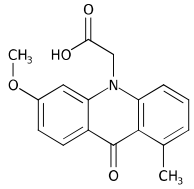
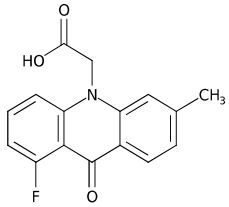
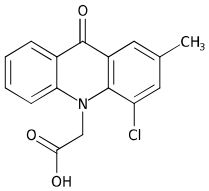
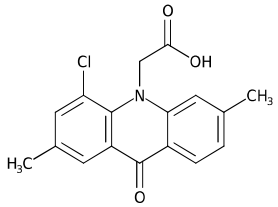
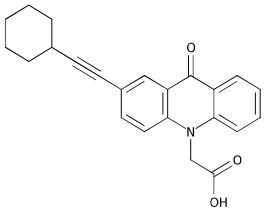
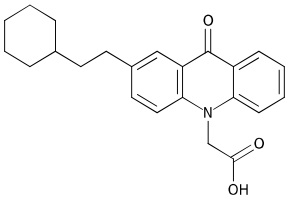
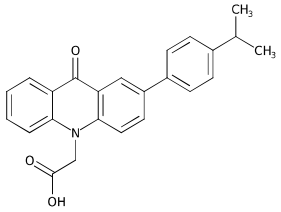
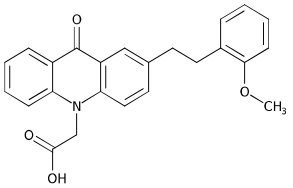
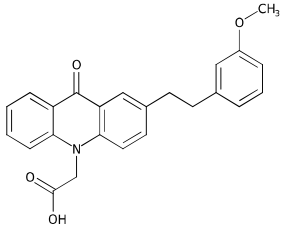
or a pharmaceutically acceptable salt or ester thereof, as a medicament for the treatment of a condition modulated by a STING protein.

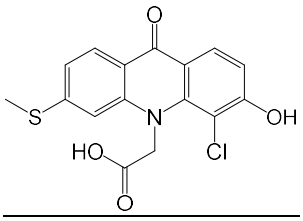
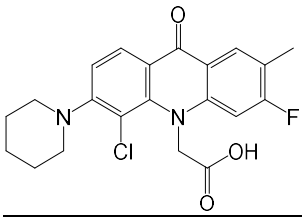
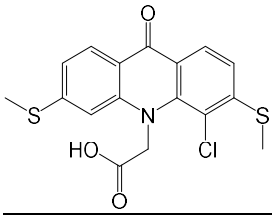
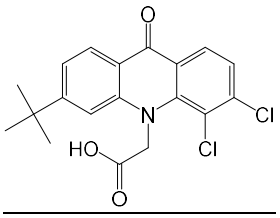
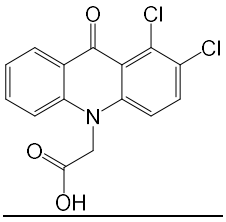
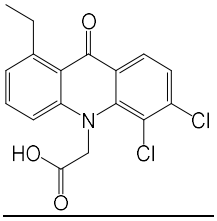
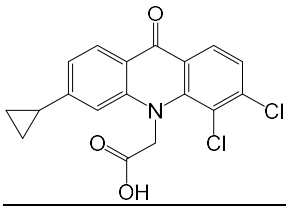
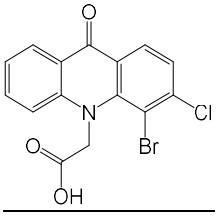
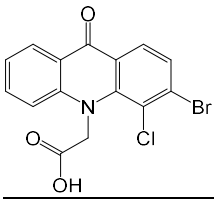
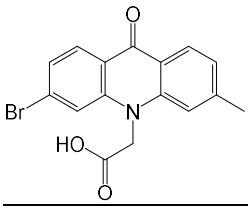
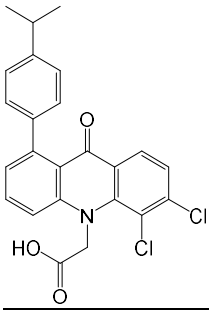
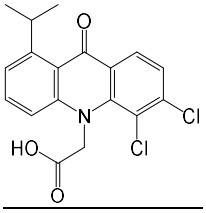
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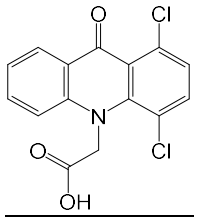
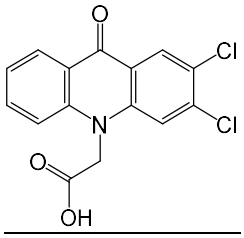
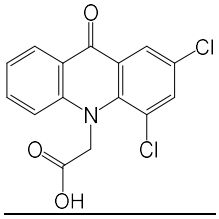
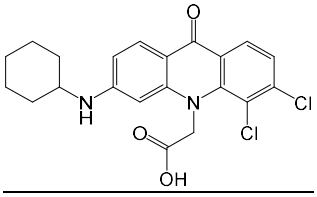
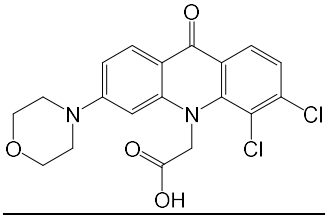
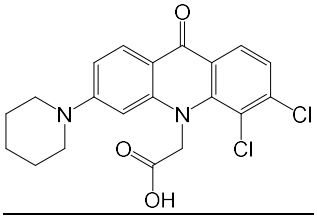
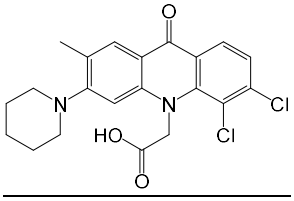
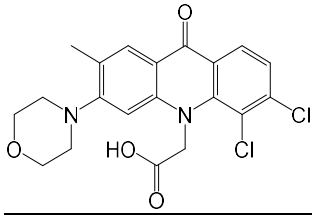
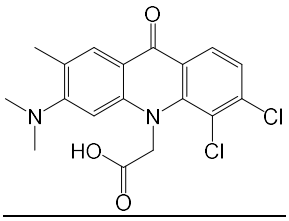
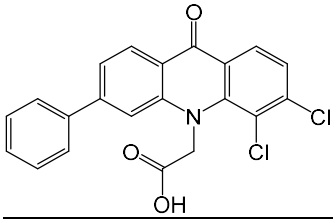
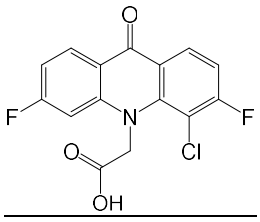
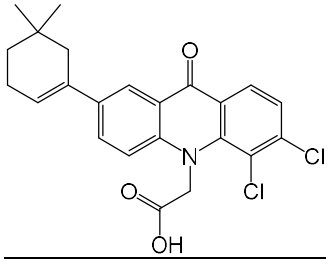
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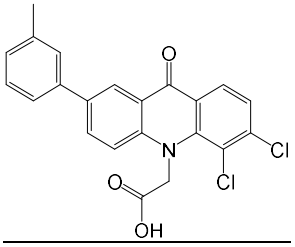
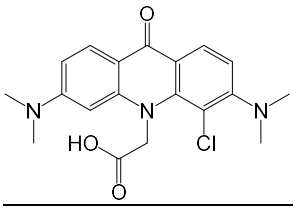
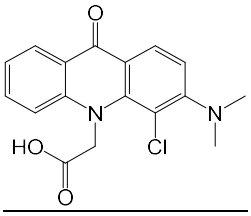
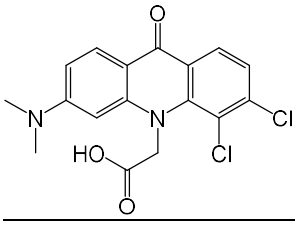
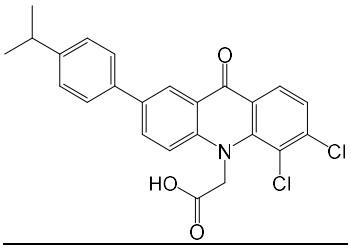
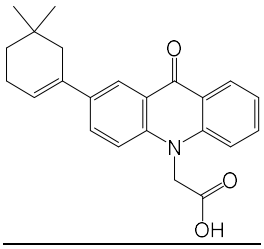
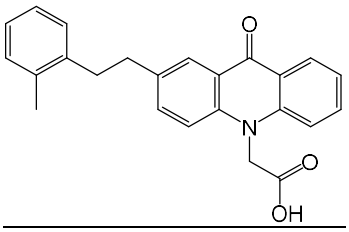
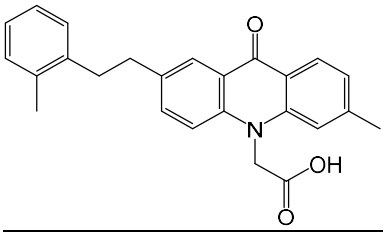
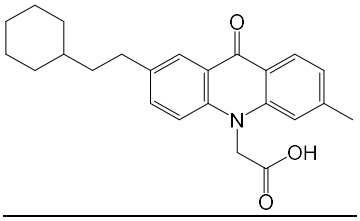
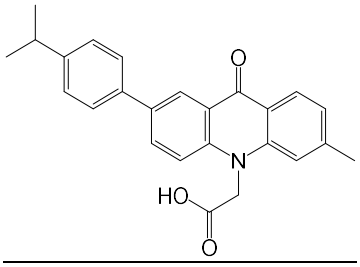
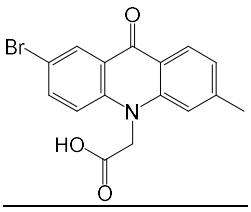
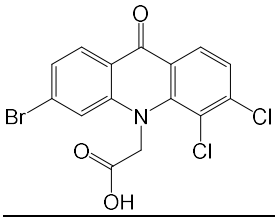
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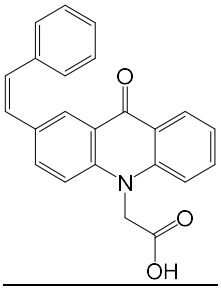
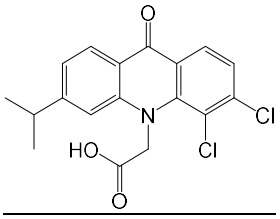
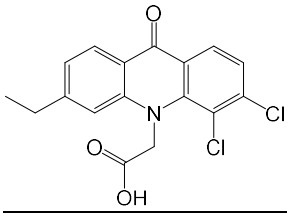
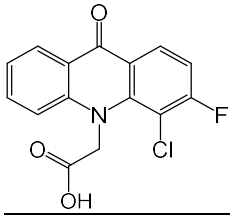
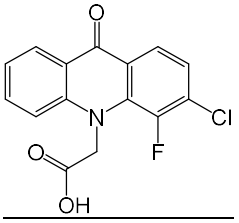
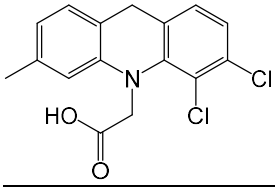
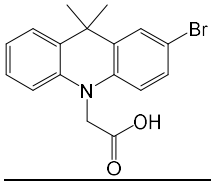
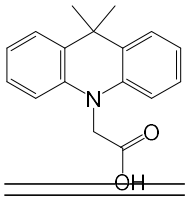
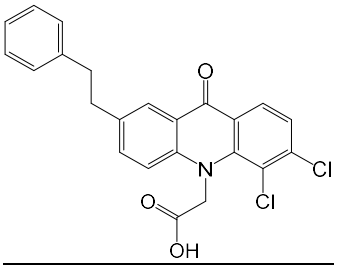
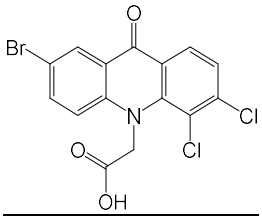
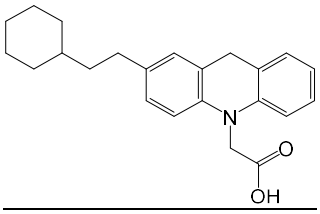
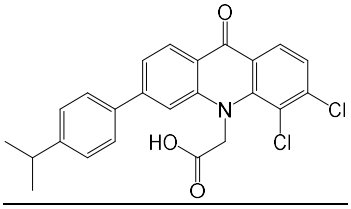
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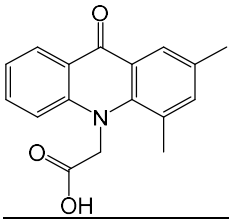
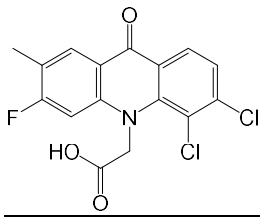
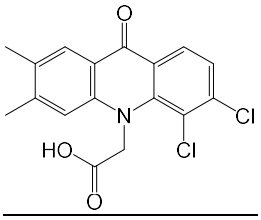
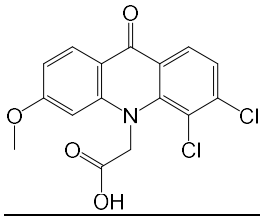
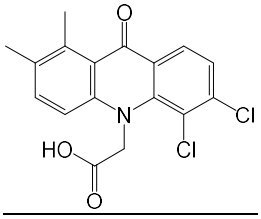
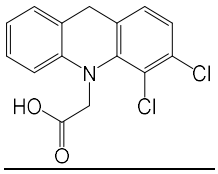
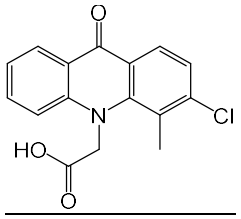
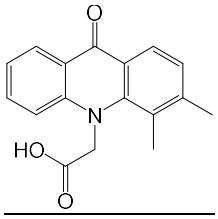
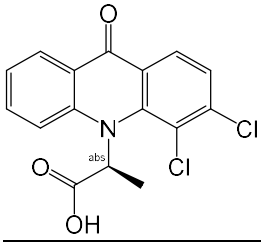
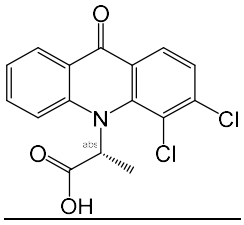
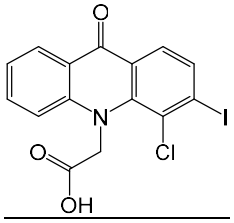
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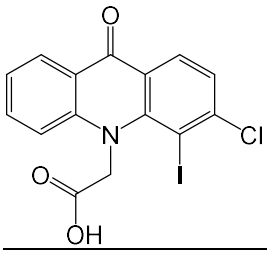
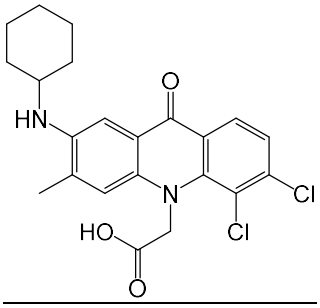
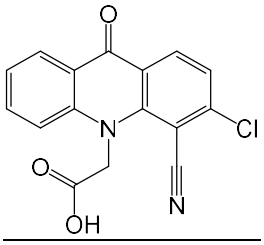
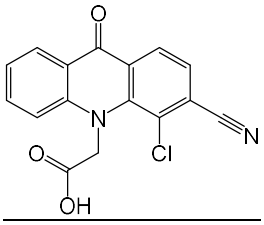
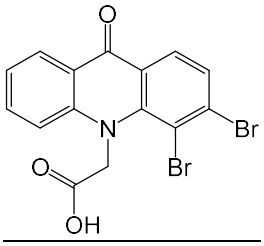
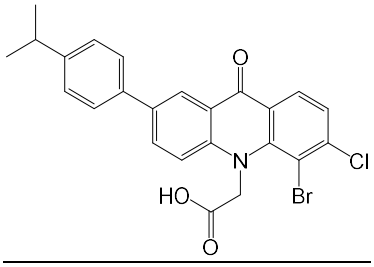
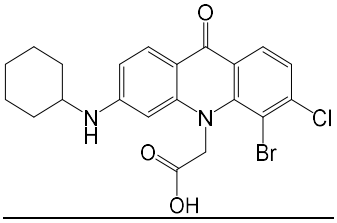
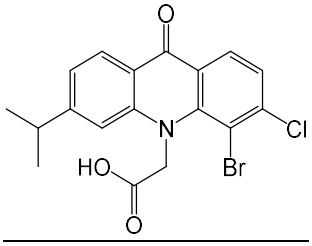
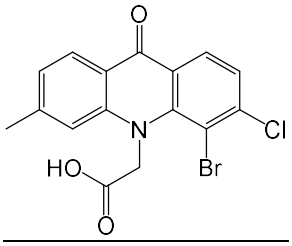
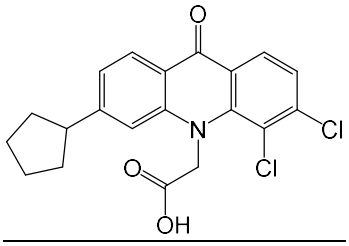
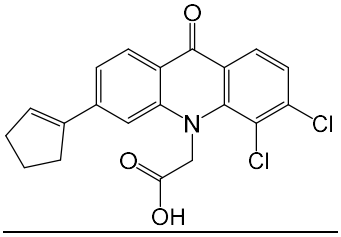
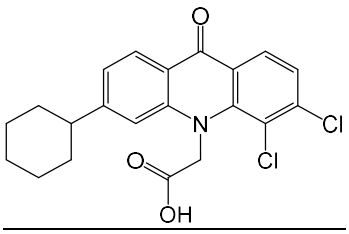
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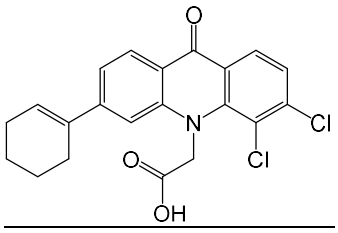
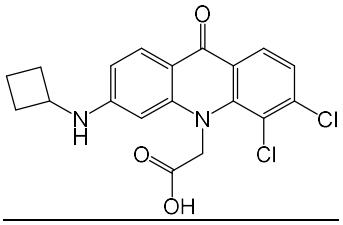
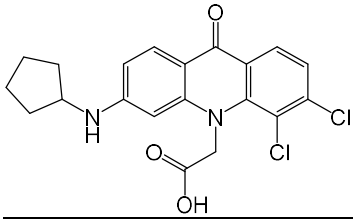
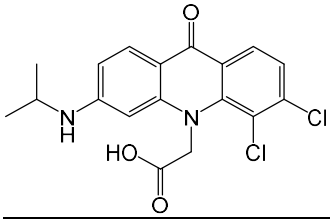
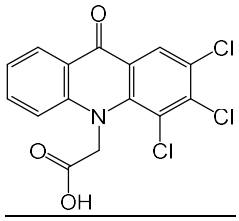
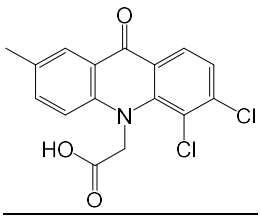
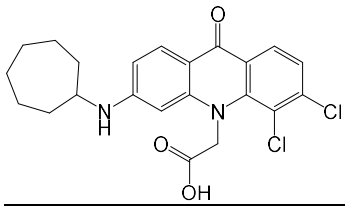
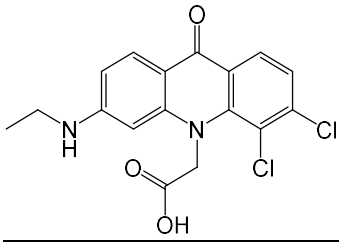
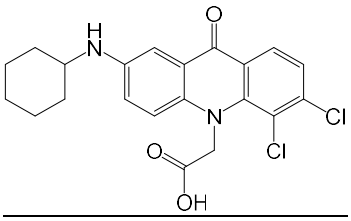
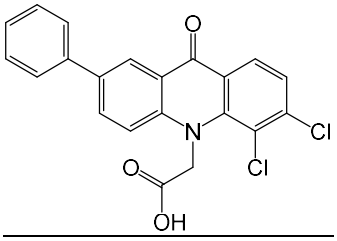
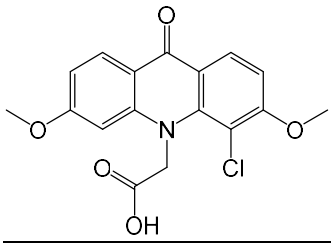
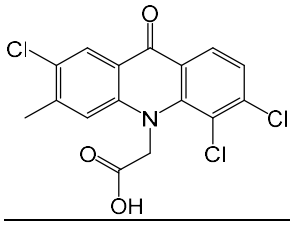
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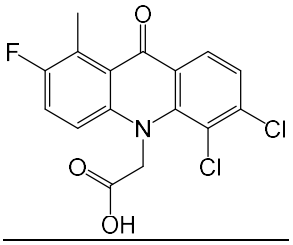
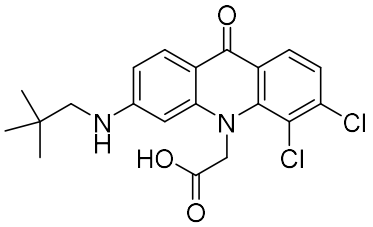
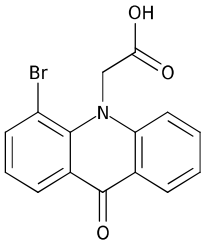
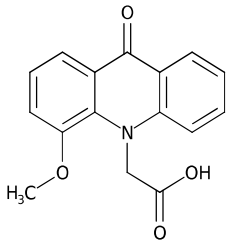
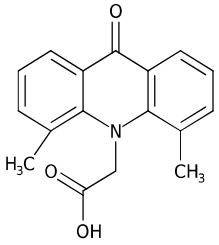
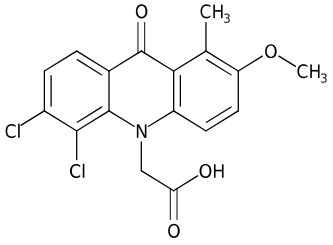
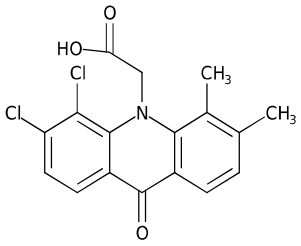
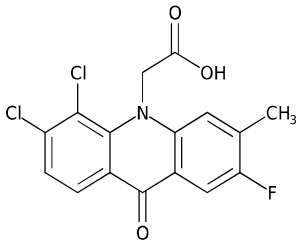
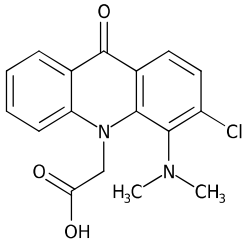
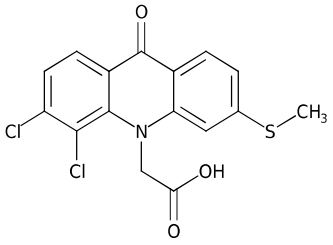
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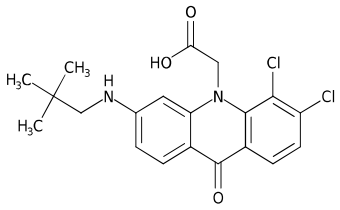
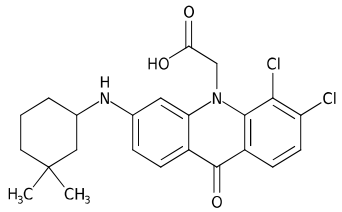
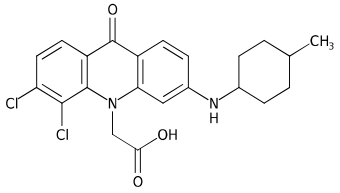
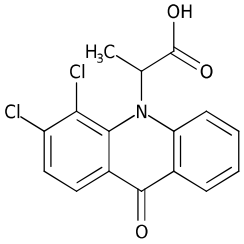
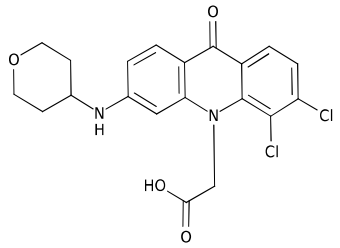
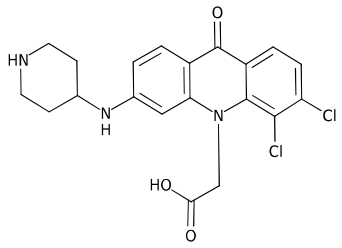
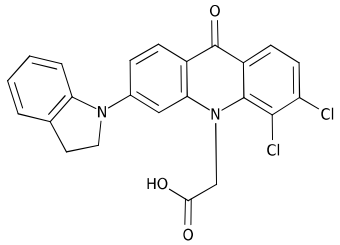
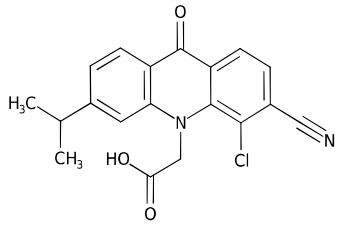
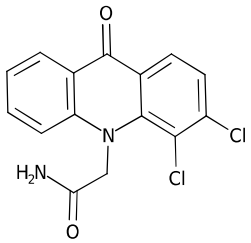
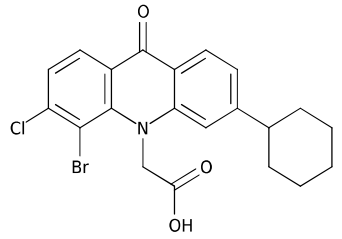
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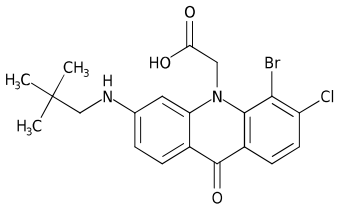
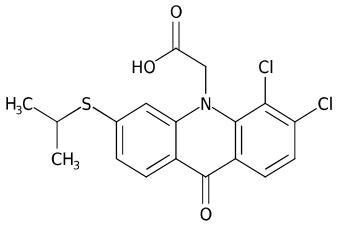
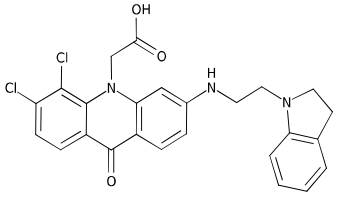
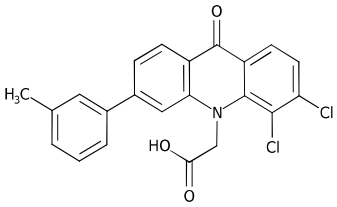
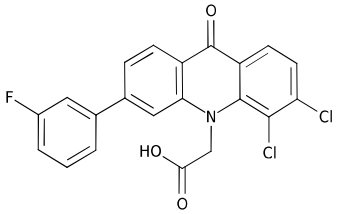
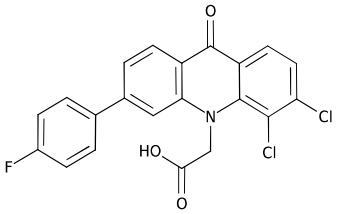
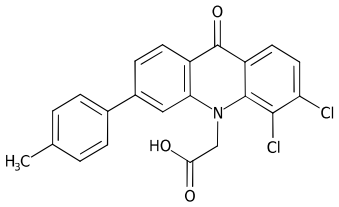
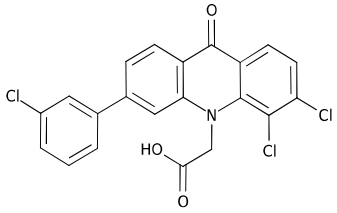
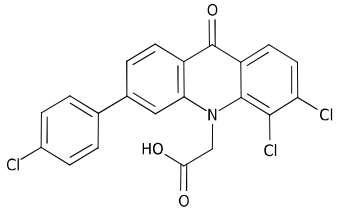
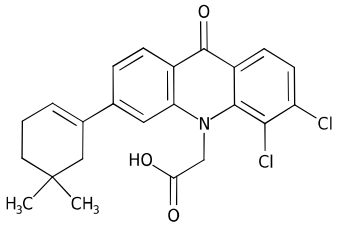
Cmpd No.	Structure	Cmpd No.	Structure
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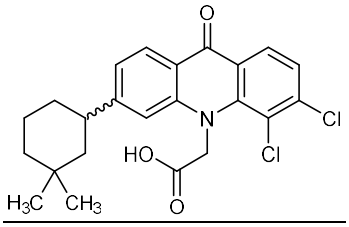
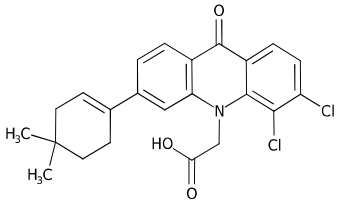
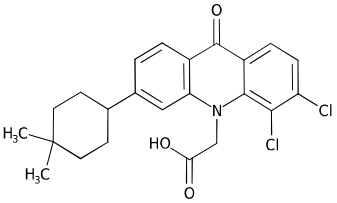
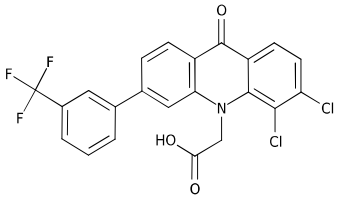
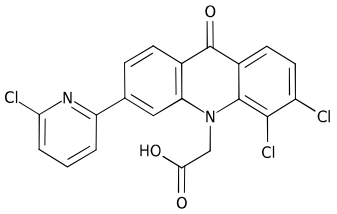
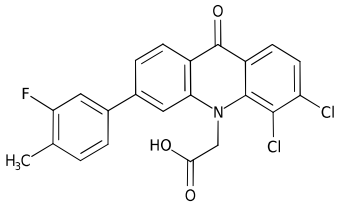
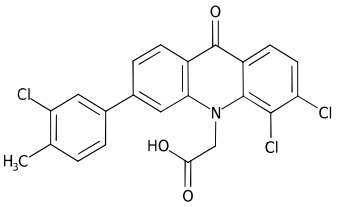
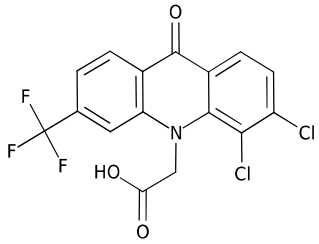
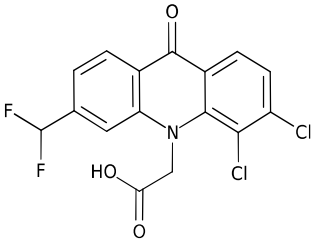
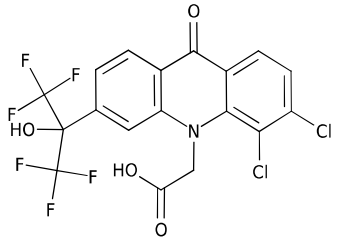
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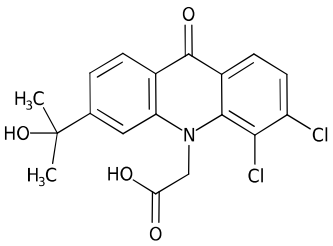
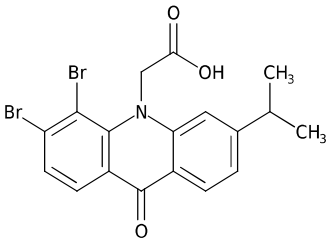
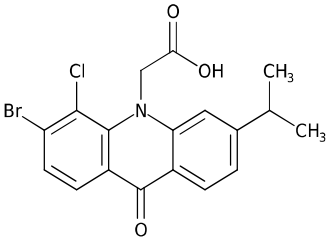
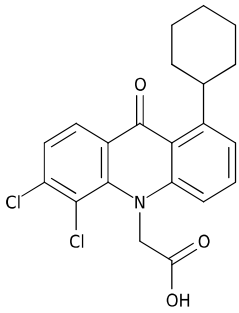
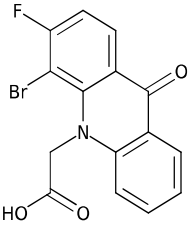
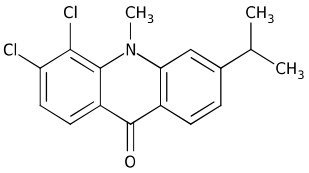
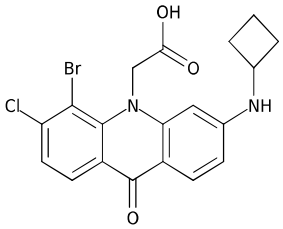
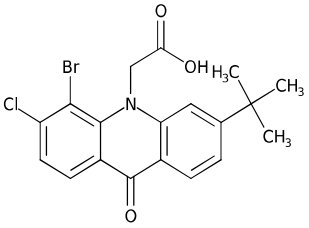
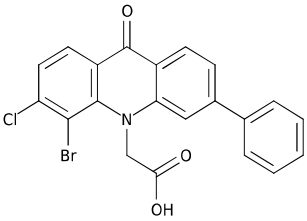
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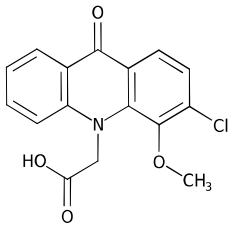
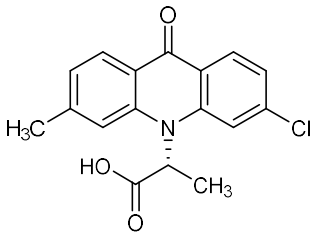
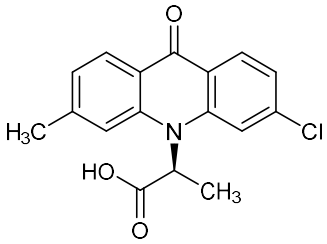
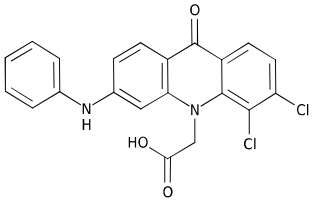
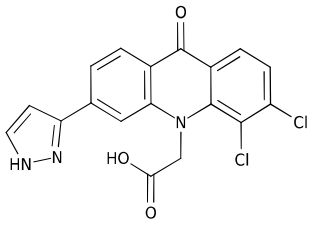
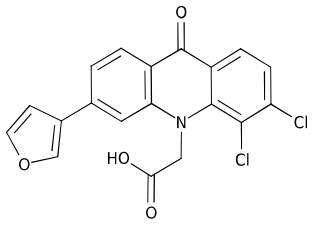
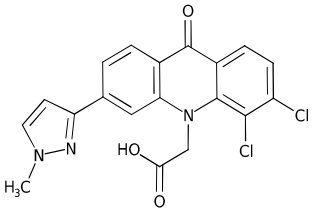
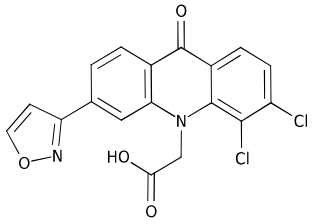
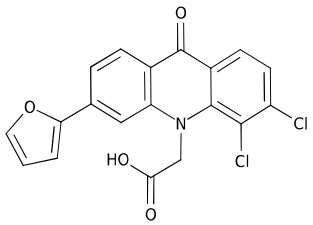
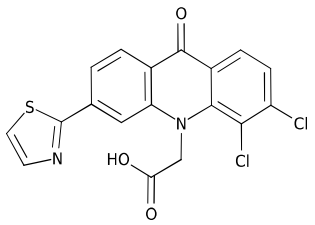
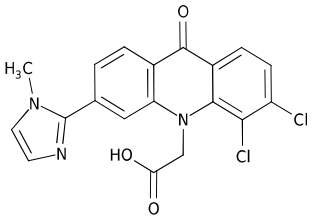
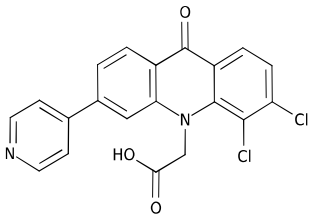
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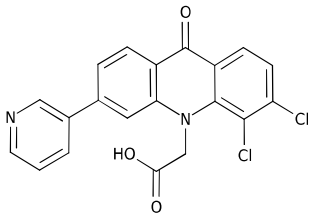
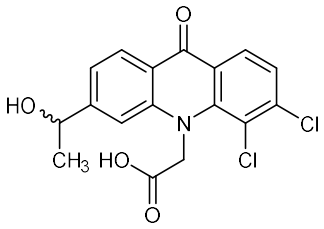
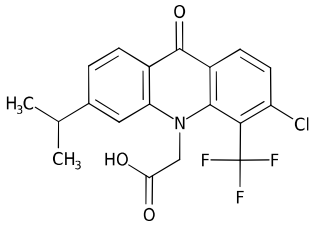
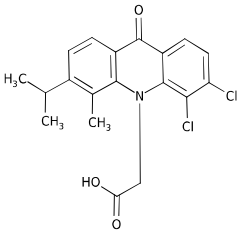
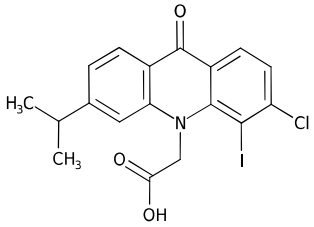
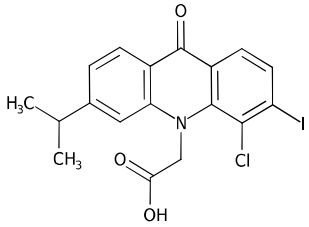
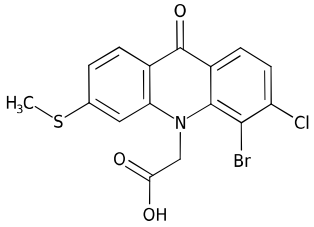
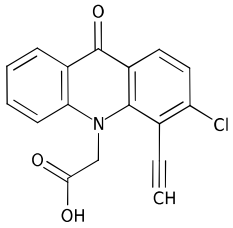
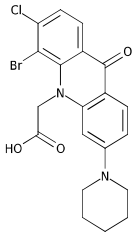
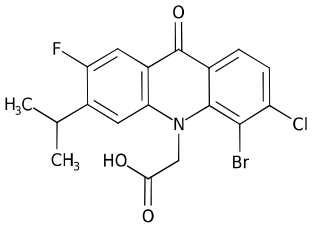
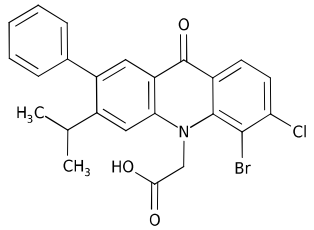
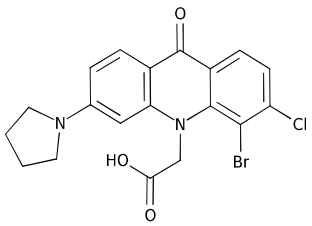
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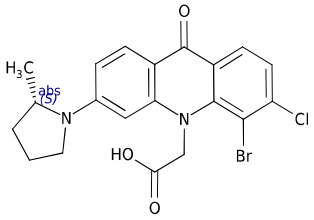
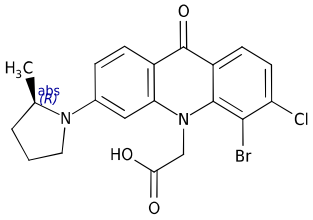
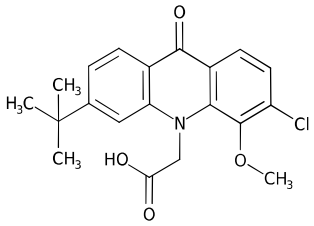
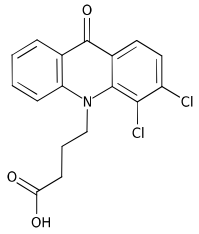
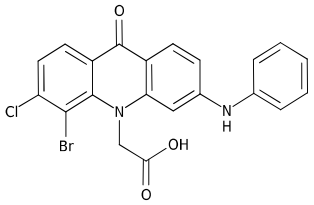
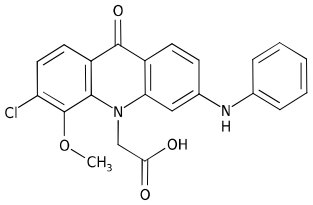
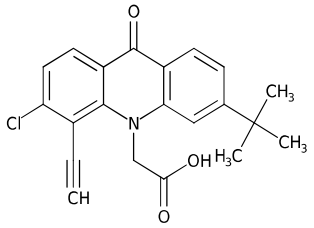
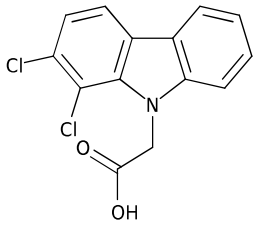
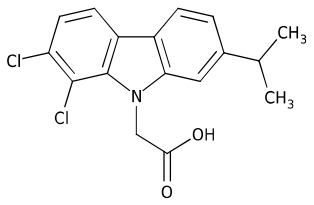
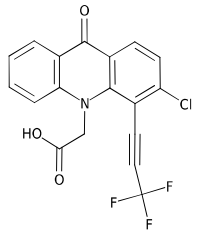
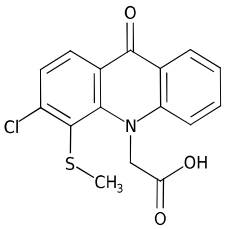
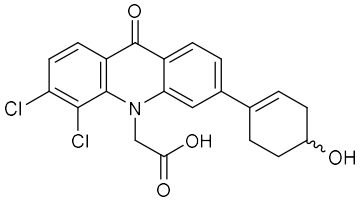
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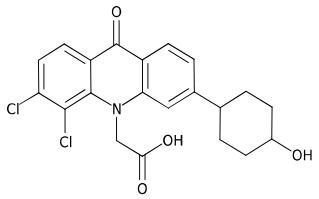
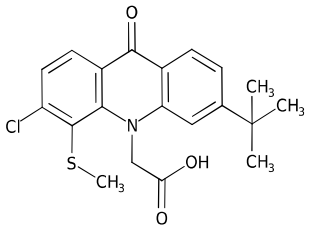
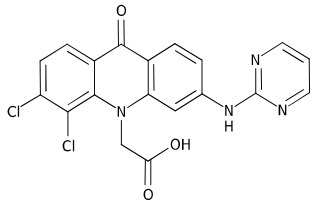
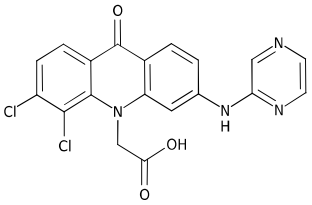
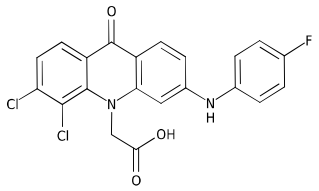
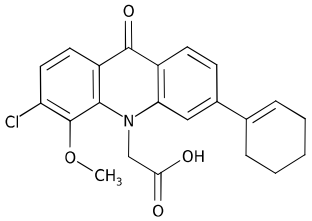
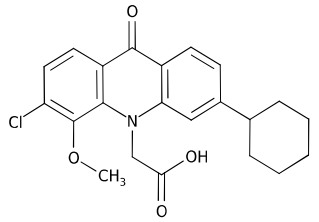
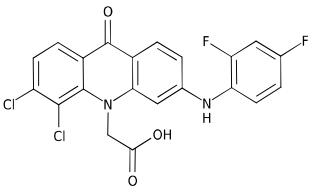
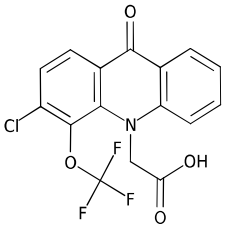
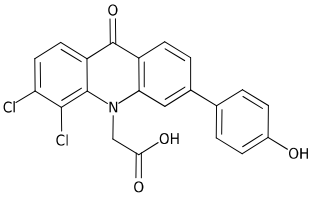
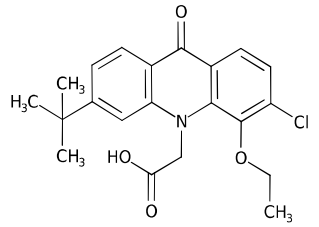
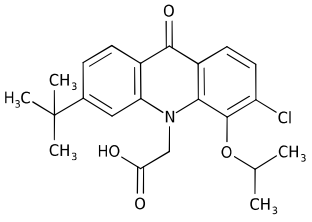
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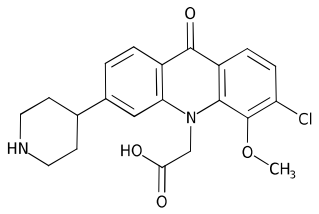
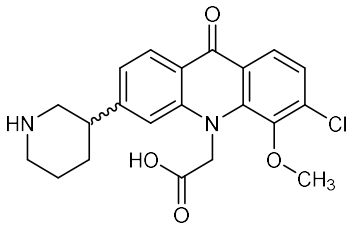
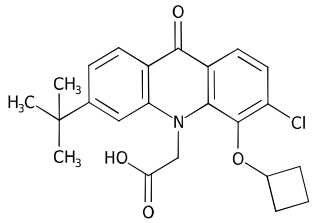
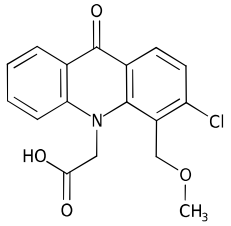
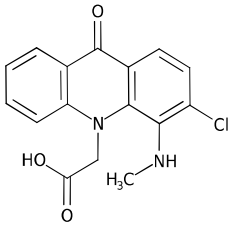
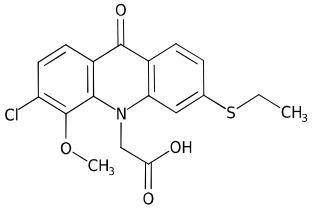
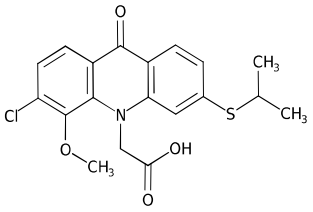
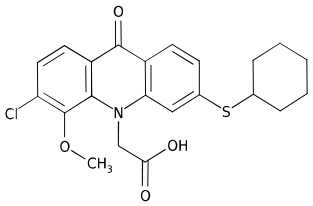
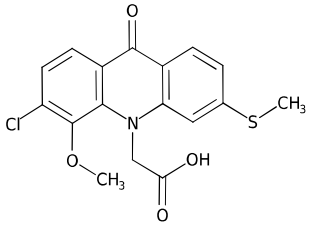
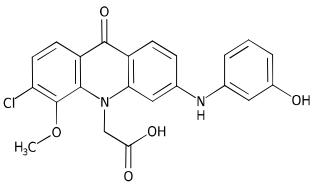
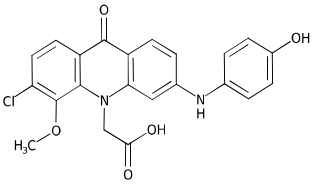
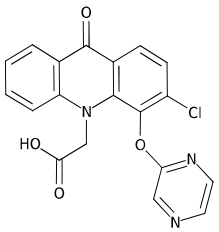
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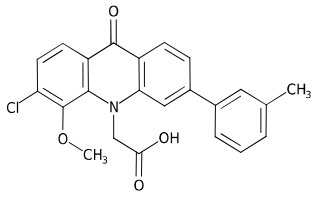
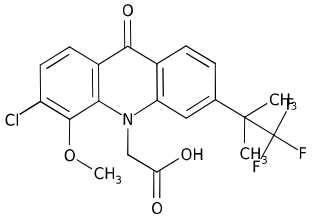
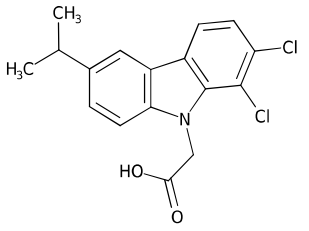
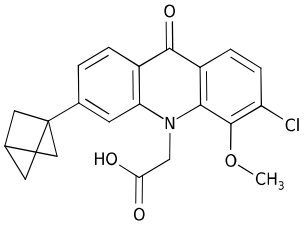
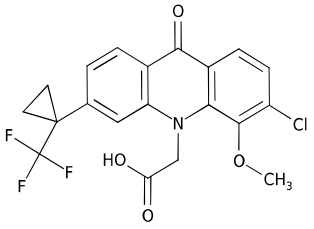
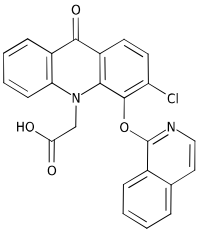
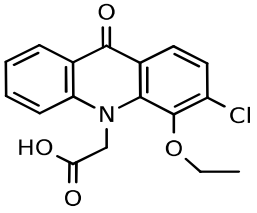
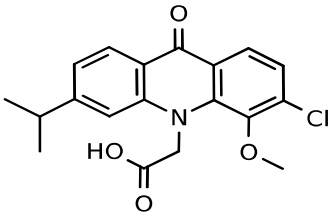
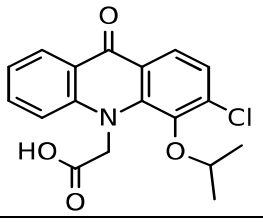
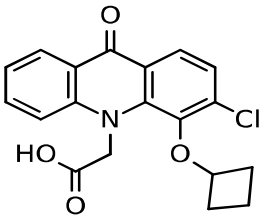
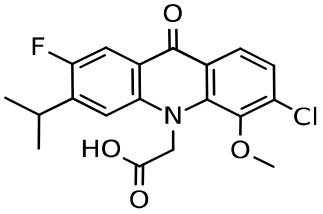
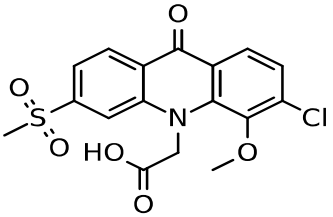
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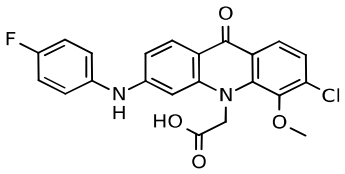
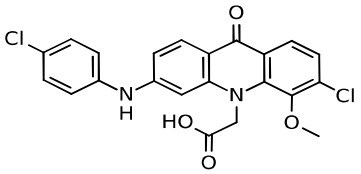
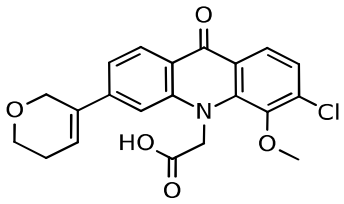
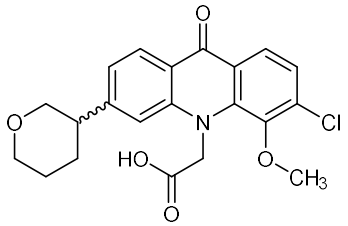
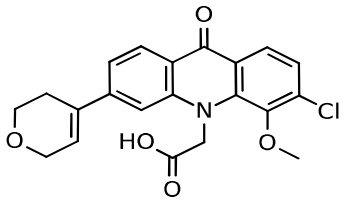
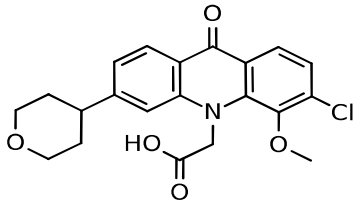
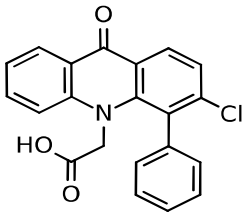
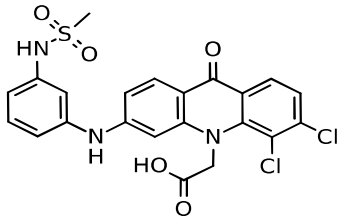
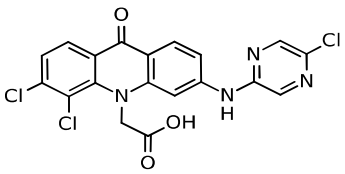
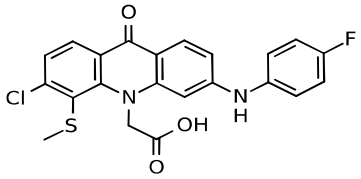
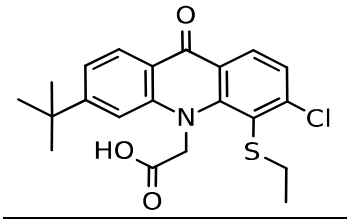
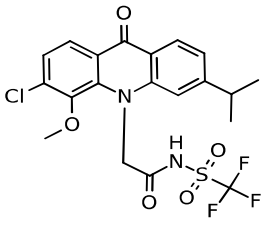
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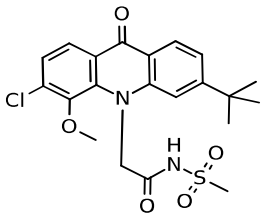
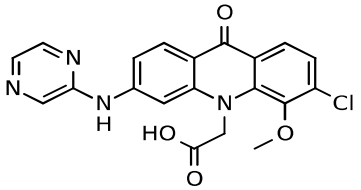
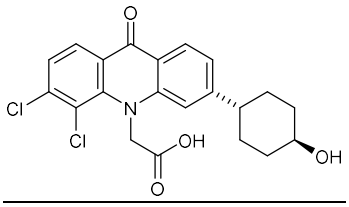
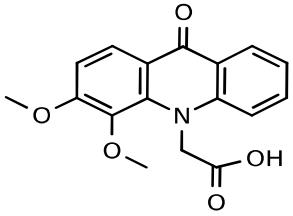
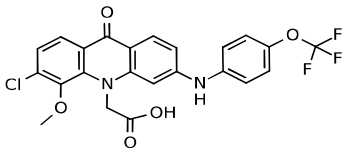
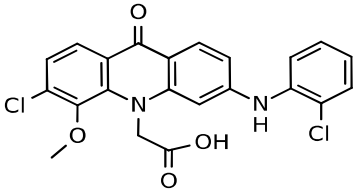
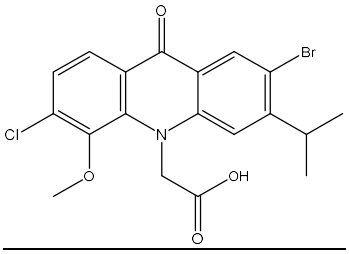
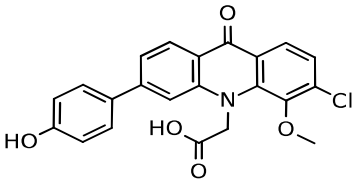
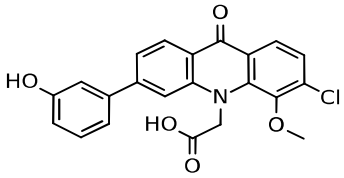
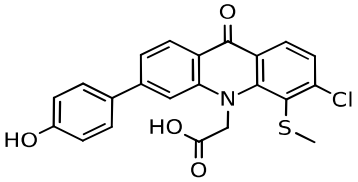
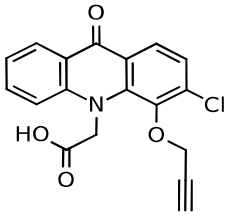
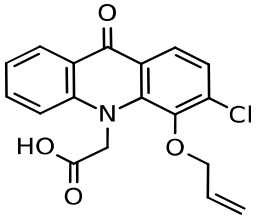
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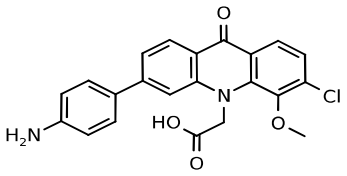
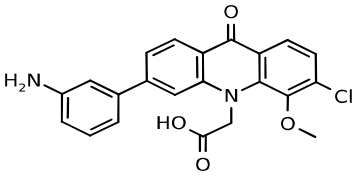
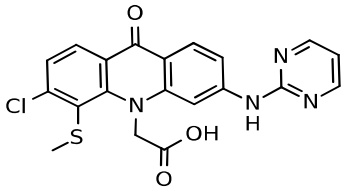
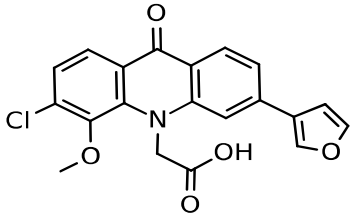
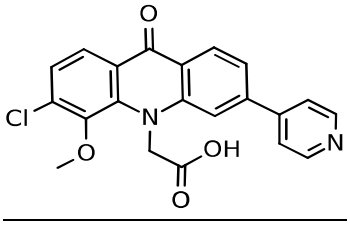
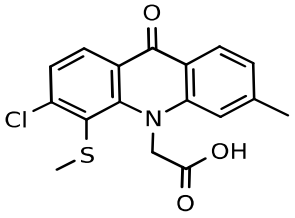
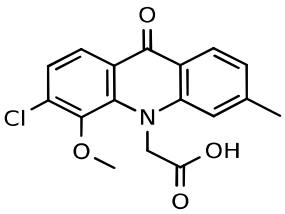
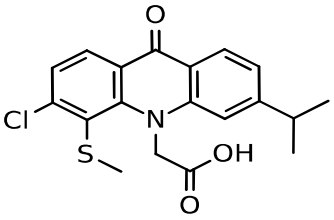
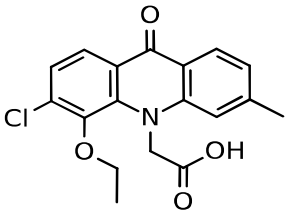
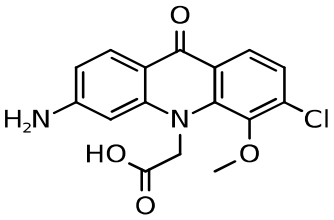
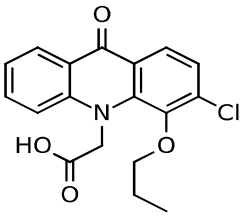
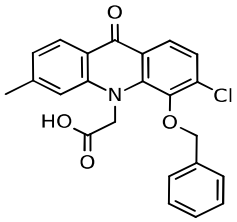
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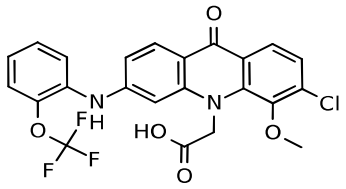
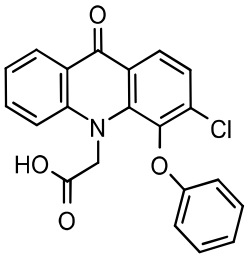
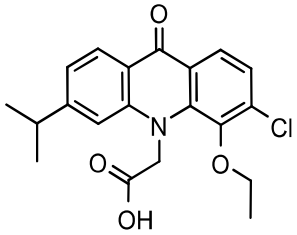
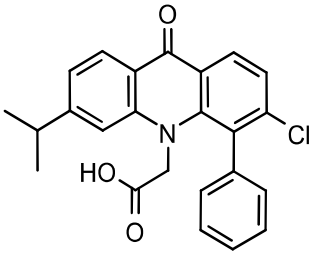
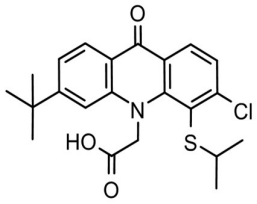
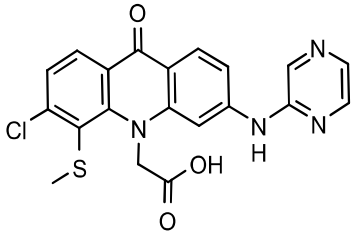
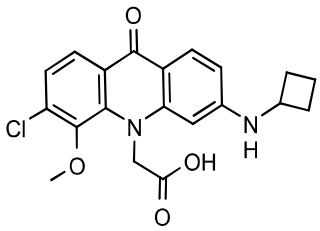
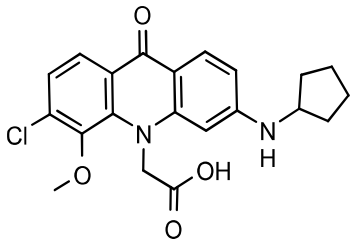
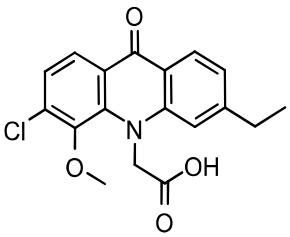
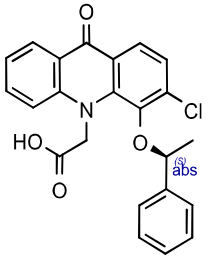
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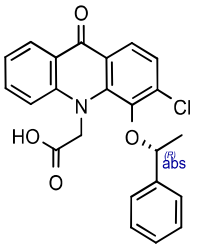
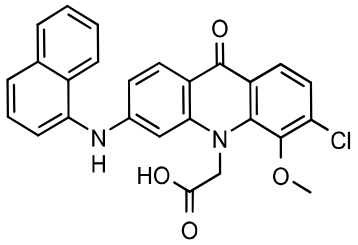
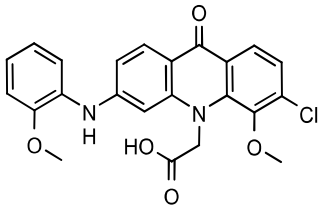
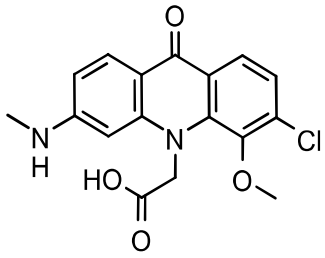
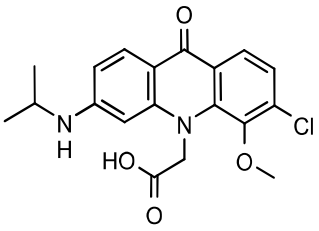
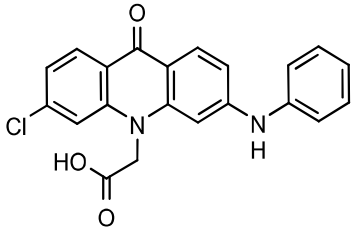
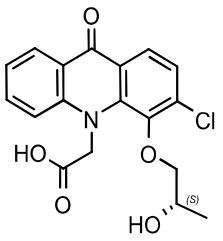
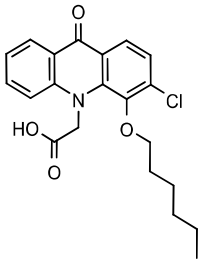
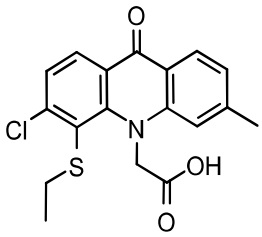
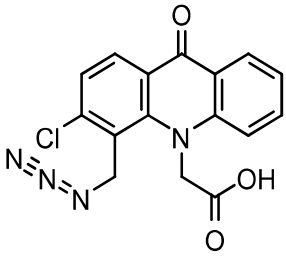
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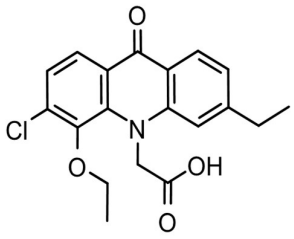
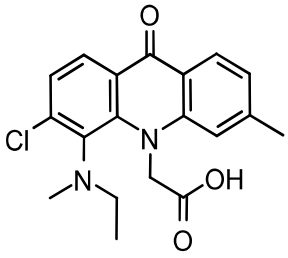
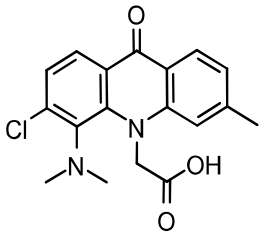
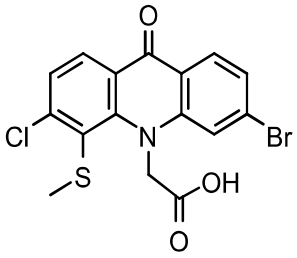
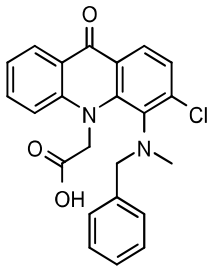
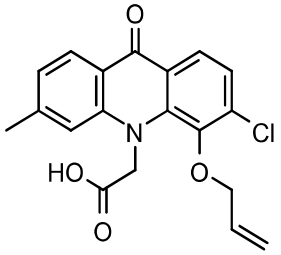
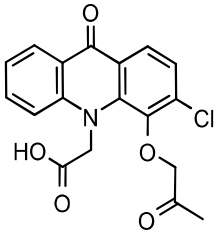
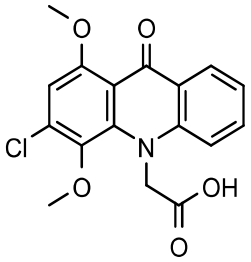
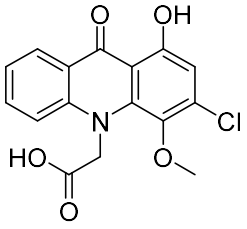
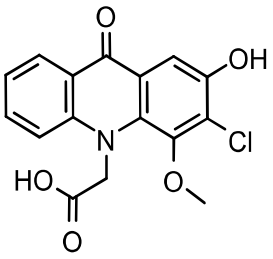
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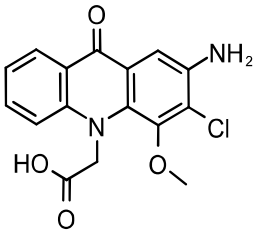
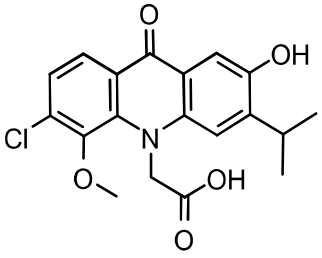
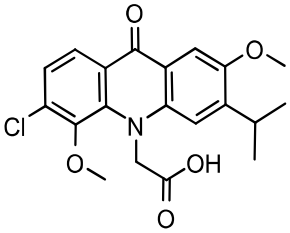
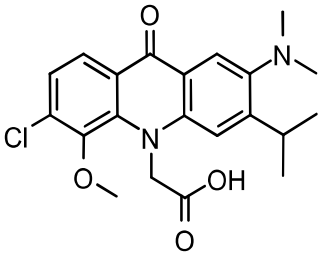
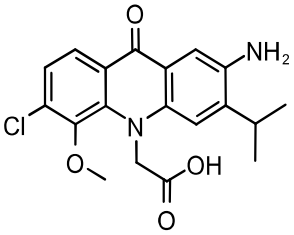
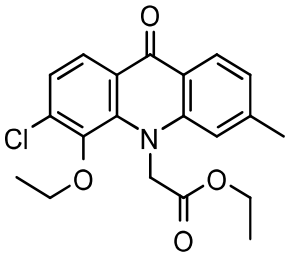
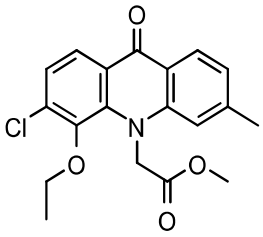
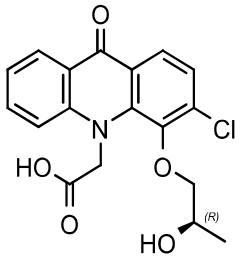
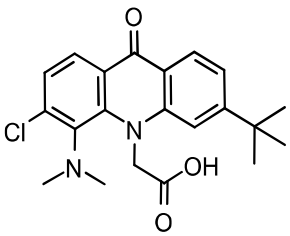
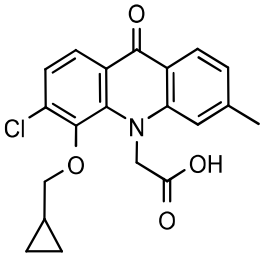
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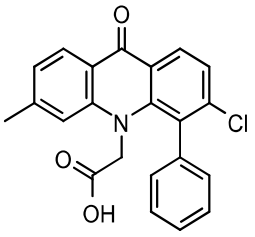
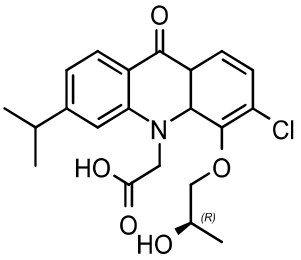
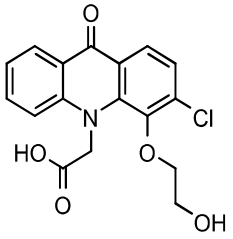
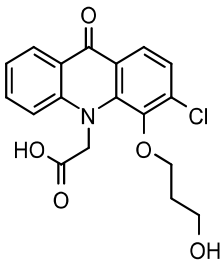
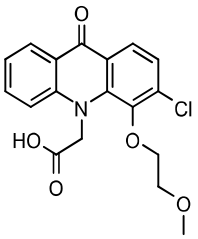
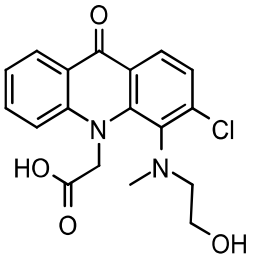
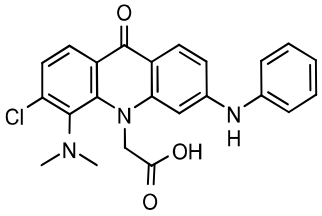
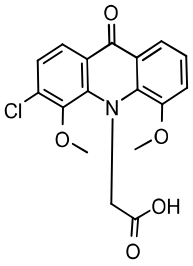
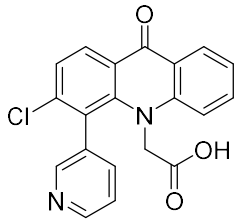
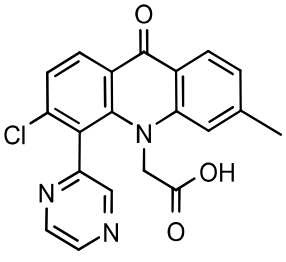
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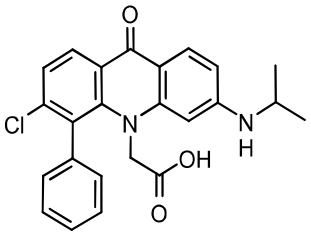
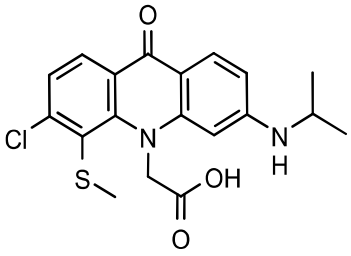
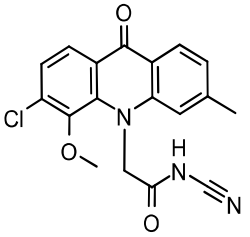
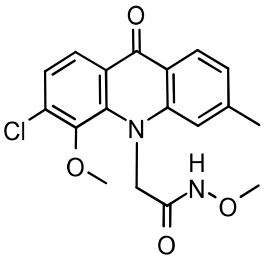
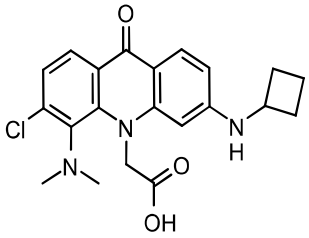
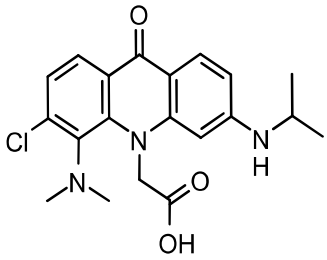
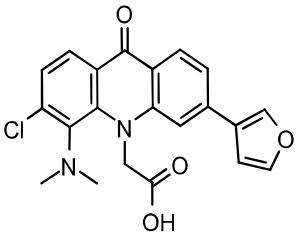
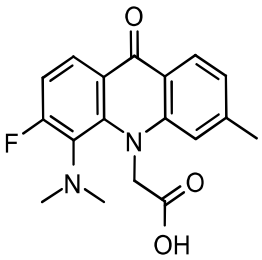
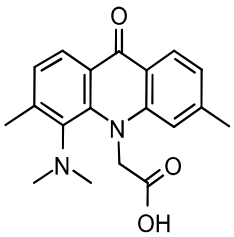
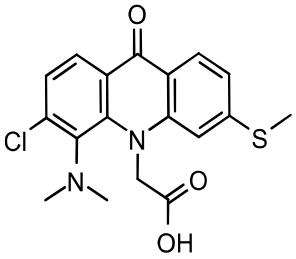
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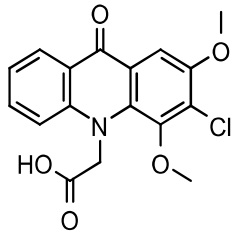
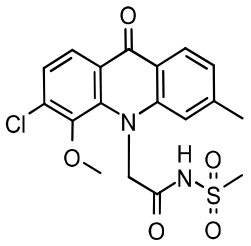
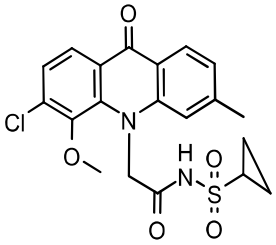
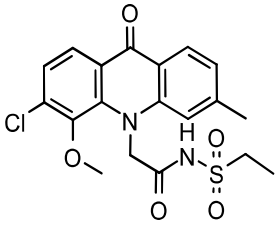
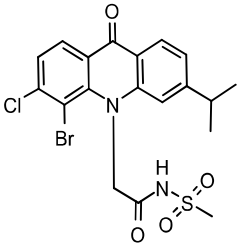
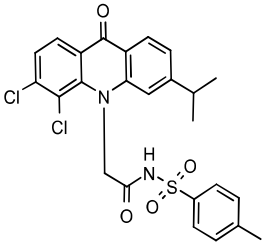
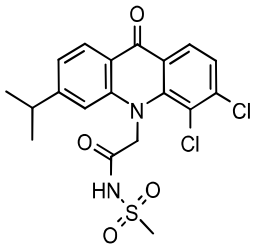
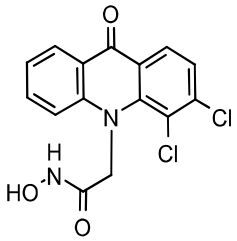
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Cmpd No.	Structure	Cmpd No.	Structure
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Cmpd No.	Structure	Cmpd No.	Structure
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Cmpd No.	Structure	Cmpd No.	Structure
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Cmpd No.	Structure	Cmpd No.	Structure
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Cmpd No.	Structure	Cmpd No.	Structure
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350		351	
352		353	

or a pharmaceutically acceptable salt or ester thereof.