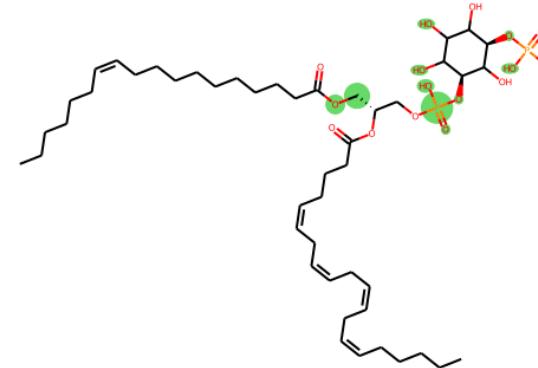


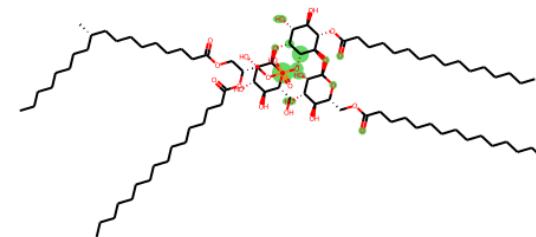
SMILES: [C@H]1C(C(C([C@H](C1O)O)O)O)OP(OC[C@H]1[COC(CC/C=C/C=C/C=C/CCCCCCCC)=O](OC(CCCCCC/C=C/CCCCCC)=O)[H])O=O

Predicted classes: phosphatidylinositol glycerophosphoinositol



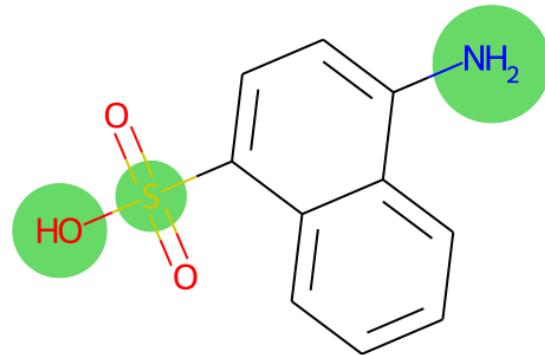
SMILES: O=C[C@H](COP(=O)(=O)OC[C@H]1C(C([C@H](C1)OP(=O)(=O)O)O)O)(OC(CCC/C=C/C=C/C=C/C=C/CCCCCC)=O)[H])C(CCCCCCCCCCC/C=CCCCCCCC)=O

Predicted classes: phosphatidylinositol  glycerophosphoinositol 



SMILES: O([C@H]1[C@H]([C@H]([C@H]([C@H]([C@H]1O[C@H]2[C@H]([C@H]([C@H](O2)COC(=O)CCCCCCCCCC)O)O)O)O[C@H]3[C@H]([C@H]([C@H]([C@H](O3)CO)O)O)O)P(=O)(O)OC[C@H](CO(CCCCCCCC[C@H](CCCCCCCC)C)=O)OC(CCCCCCCCCCCCCC)=O

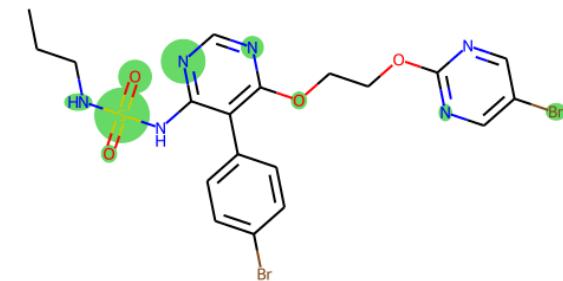
Predicted classes: glycoglycerolipid  glycoprophospholipid  phosphatidylinositol  glycerophosphoinositol 



SMILES: Nc1ccc(c2ccccc12)S(O)(=O)=O

Atoms: NCCCCCCCCCSOOO

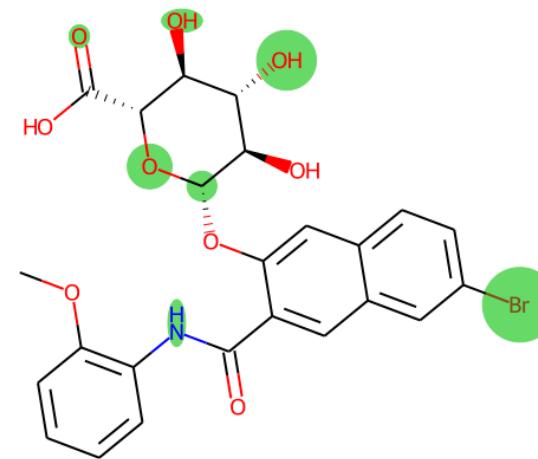
Predicted classes: arenesulfonic acid organosulfonic acid



SMILES: CCCNS(=O)(=O)Nc1ncncc(OCCOc2ncc(Br)cn2)c1-c1ccc(Br)cc1

Atoms: CCCNSOONCNCNCOCCOCNCCBrCNCCCCBrCC

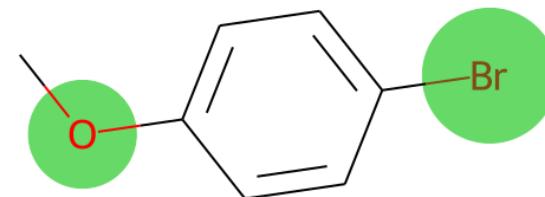
Predicted classes: organobromine compound bromine molecular entity sulfuric acid derivative



SMILES: [C@H]1([C@H]([C@H](O)[C@H]([C@H](O)C(O)=O)O)OC=2C(=CC=3C=C(C=CC3C2)Br)C(=O)NC=4C(=CC=CC4)OC

Atoms: CCCOCCOCOOOOCCCCCCCCCBrCONCCCCCCCO

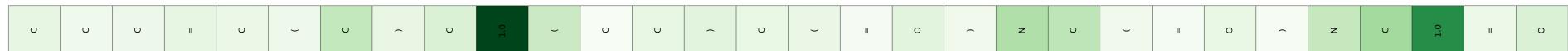
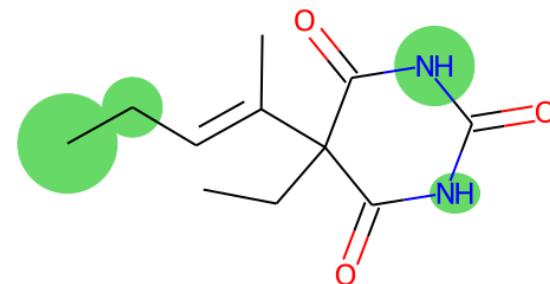
Predicted classes: glucosiduronic acid glycosiduronic acid carbohydrate acid derivative organobromine compound bromine molecular entity



SMILES: COc1ccc(Br)cc1

Atoms: COCCCCBrCC

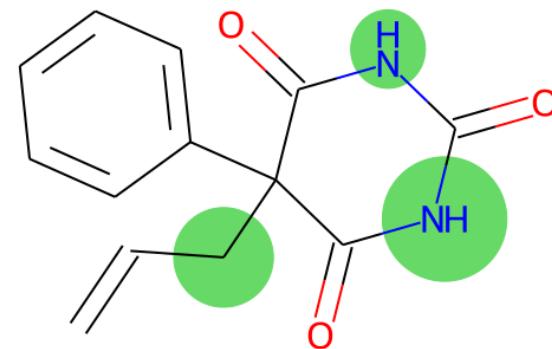
Predicted classes: monomethoxybenzene ✕ organobromine compound ✕ bromine molecular entity ✕



SMILES: CCC=C(C)C1(CC)C(=O)NC(=O)NC1=O

Atoms: CCCCCCCCNC(=O)N

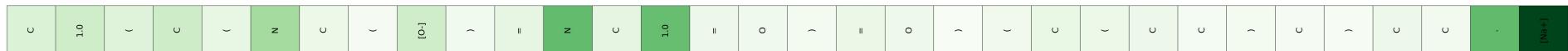
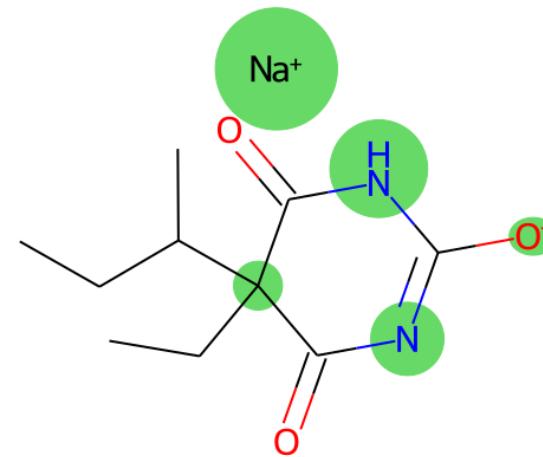
Predicted classes: barbiturates ✕ pyrimidone ✕



SMILES: C(C=C)C1(C(=O)NC(NC1=O)=O)C2=CC=CC=C2

Atoms: CCCCCONCNCOOCCCCCC

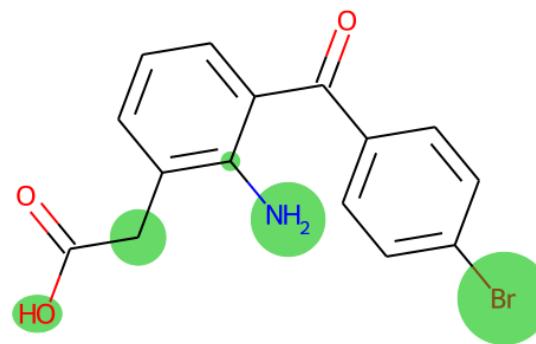
Predicted classes: barbiturates ✘ pyrimidone ✘



SMILES: C1(C(NC([O-])=NC1=O)=O)(C(CC)CC.[Na+]

Atoms: CCNCONCOOC₆H₅CCNa

Predicted classes: barbiturates ✘ pyrimidone ✘



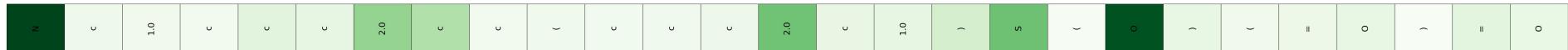
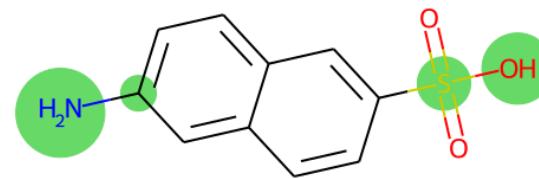
n	c	1.0	c	-	c	c	(o)	=		o)	c	c	c	c	1.0	c	-		o)	c	c	c	c	1.0	c	c	c	c	Br)	c	c	1.0
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SMILES: Nc1cc(CC(=O)=O)cccc1C(=O)c1ccc(Br)cc1

Atoms: NCCCCOCCCCCCBrCC

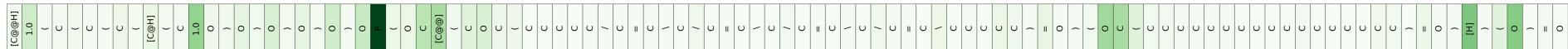
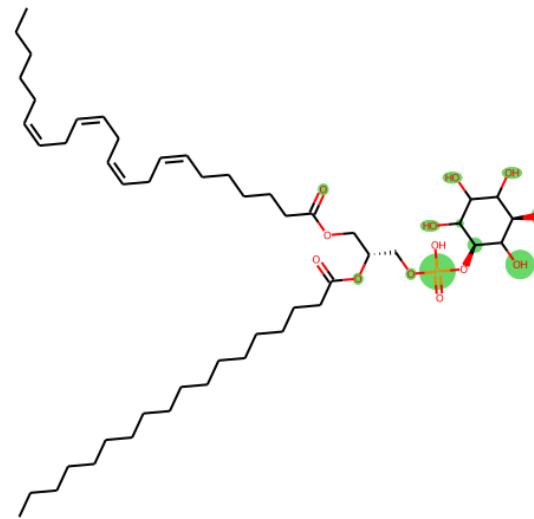
Predicted classes:

substituted aniline ✖anilines ✖organobromine compound ✖bromine molecular entity ✖

SMILES: Nc1ccc2cc(c1)S(=O)(=O)O

Atoms: NCCCCCCCCCCSOOO

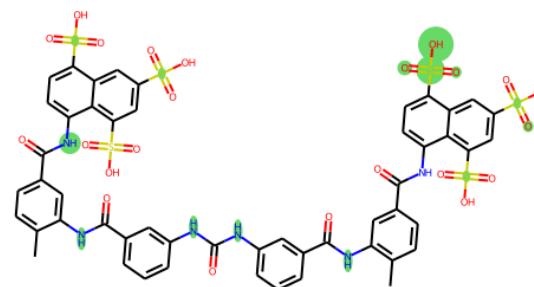
Predicted classes: arenesulfonic acid organosulfonic acid



SMILES: [C@H]1(C(C(C([C@H](C1O)O)O)O)OP(OC[C@H](COC(CCCCCC/C=C/C/C=C/C=C\CCCC)=O)(OC(CCCCCC/C=C/C/C=C/C=C\CCCC)=O)[H])(O)=O

Atoms: CCCCCCOOOOOPOCCOCCCCCCCCCCCCCCCCCCCCCCOCCCCCCCCCCCCCCCCCOOO

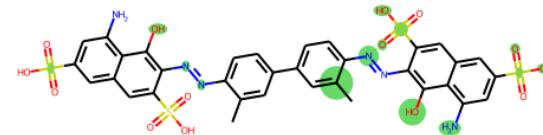
Predicted classes: phosphatidylinositol ✕ glycerophosphoinositol ✕



SMILES: C12=C(C=C(C=C1C(=CC=C2NC(C3=CC=C(C(NC(C=4C=CC=C(C(NC(NC5=CC=CC(C(NC(=6C=CC=C(C(NC=7C8=C(C=C(C=C8C(=CC7)S(O)(=O)=O)S(O)(=O)=O)S(O)(=O)=O)C6)C)=O)=C5)=O)C4)=O)=C3)C)=O)S(O)(=O)=O)S(O)(=O)=O)S(O)(=O)=O

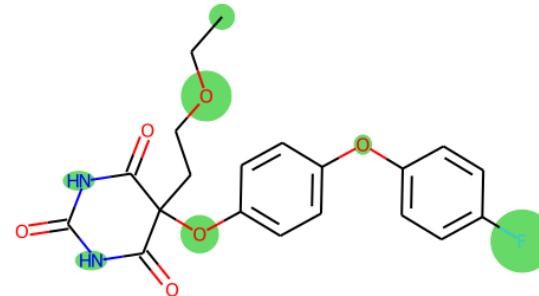
Atoms: CCCCCCCCCNCCCCCNCCCCCNCCCCCNCCCCCCCCS000S000S000OCOCOCOCOS000S000S000

Predicted classes: arenenesulfonic acid organosulfonic acid



SMILES: Cc1cc(ccc1\N=N\c1c(O)c2c(N)cc(cc2cc1S(O)(=O)=O)S(O)(=O)=O)-c1ccc(\N=N\c2c(O)c3c(N)cc(cc3cc2S(O)(=O)=O)S(O)(=O)=O)c(C)c1

Predicted classes: azo compound hydroxynaphthalene arenesulfonic acid organosulfonic acid

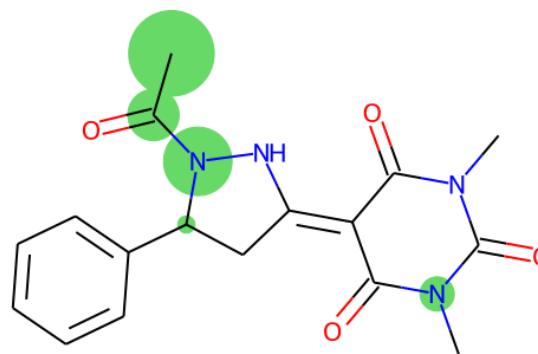


c	c	o	c	c	c	1.0	(o	c	c	c	c	c	(o	c	c	c	3.0	c	c	c	(f)	c	c	3.0	c	c	2.0)	c	(=	o)	n	c	(=	o)	n	c	1.0	=	o
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SMILES: CCOCCC1(Oc2ccc(Oc3ccc(F)cc3)cc2)C(=O)NC(=O)NC1=O

Atoms: CCOCCCOCCCCOCCCCFCCCCCONCONCO

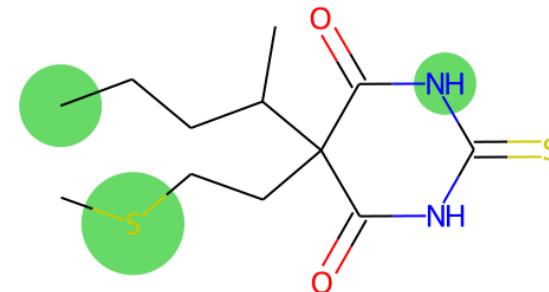
Predicted classes: barbiturates ✘ pyrimidone ✘



SMILES: CC(=O)N1C(CC(=C2C(=O)N(C(=O)N(C2=O)C)O)N1)C3=CC=CC=C3

Atoms: CCONCCCCONCONCOCCNCCCCC

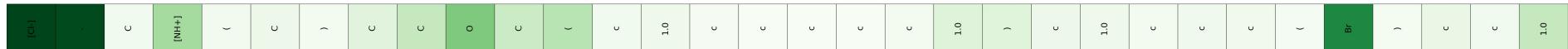
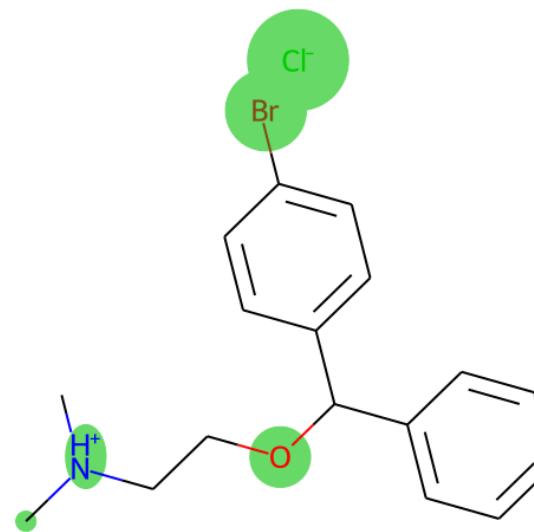
Predicted classes: barbiturates ✕ pyrimidone ✕



SMILES: CCCC(C)C1(CCSC)C(=O)NC(=S)NC1=O

Atoms: CCCCCCCSCCONCSNCO

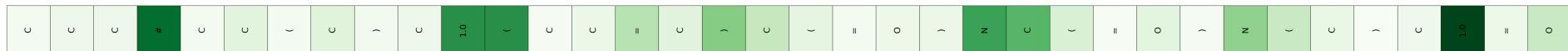
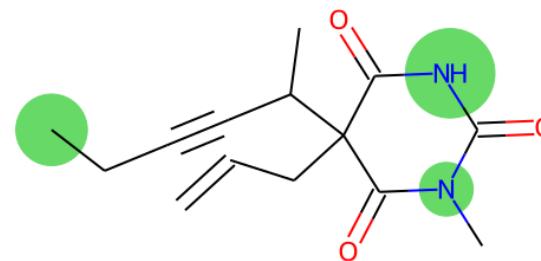
Predicted classes: barbiturates pyrimidone



SMILES: [Cl-].[NH+](C)CCOC(c1ccccc1)c1ccc(Br)cc1

Atoms: C1NCCCCCCCCCCCCBrCC

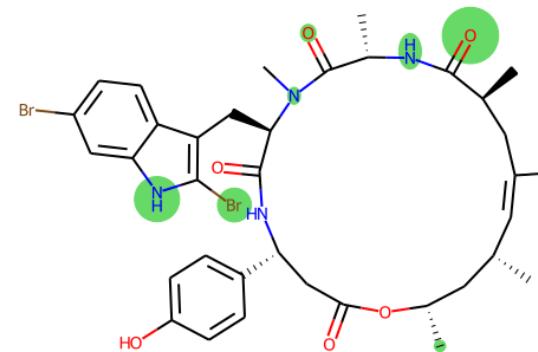
Predicted classes: organobromine compound ✕ hydrochloride ✕ bromine molecular entity ✕ organic chloride salt ✕ chloride salt ✕ organic halide salt ✕ halide salt ✕



SMILES: CCC#CC(C)C1(CC=C)C(=O)NC(=O)N(C)C1=O

Atoms: CCCCCCCCCCONCONCO

Predicted classes: barbiturates ✘ acetylenic compound ✘ pyrimidone ✘



SMILES: C[C@H]1C[C@H](C)C=C(C)C[C@H](C)C(=O)N[C@H](C)C(=O)N(C)[C@H](Cc2c(Br)[nH]c3cc(Br)ccc23)C(=O)N[C@H](CC(=O)O1)c1ccc(O)cc1
Atoms: CCCCCCCCCCCC CONCCCONCCCCBrNCCCBrCCCCONCCCOCCCCOCC

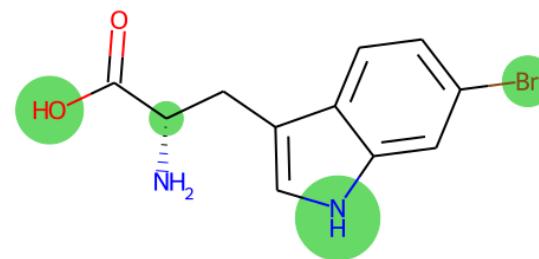
Predicted classes:

cyclodepsipeptide ✖

depsipeptide ✖

organobromine compound ✖

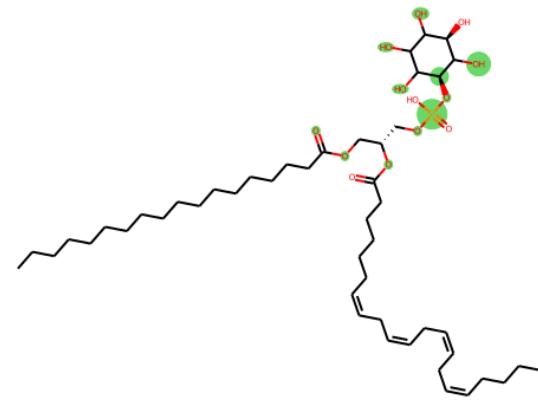
bromine molecular entity ✖



SMILES: N[C@H](Cc1c[nH]c2cc(Br)ccc12)C(=O)O

Atoms: NCCCCNCCCCBrCCCCOO

Predicted classes: non-proteinogenic L-alpha-amino acid organobromine compound L-alpha-amino acid bromine molecular entity non-proteinogenic alpha-amino acid alpha-amino acid non-proteinogenic amino acid



Predicted classes: phosphatidylinositol glycerophosphoinositol

Fe

[Fe]

SMILES: [Fe]

Atoms: Fe

Predicted classes:

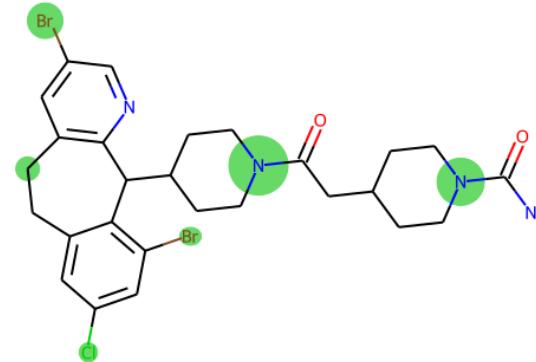
iron molecular entity

iron group molecular entity

elemental molecular entity

d-block molecular entity

transition element molecular entity

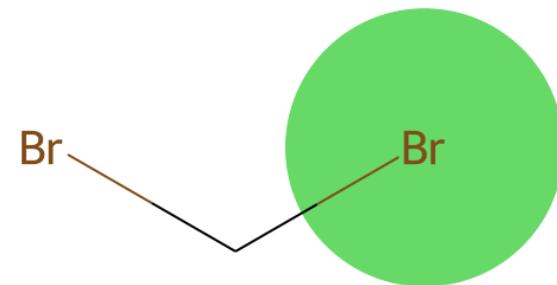


C 1.0
C 2.0
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N
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C
(
O
)
Br
)
Cl

SMILES: C=12CCC=3C=C(C=C(C3C(C1N=CC(=C2Br)C4CCN(CC4)C(=O)CC5CCN(CC5)C(N)=O)Br)Cl

Atoms: CCCCCCCCCCNCCCCBrCCCCNCCCOCCCCNCCCCNOBrCl

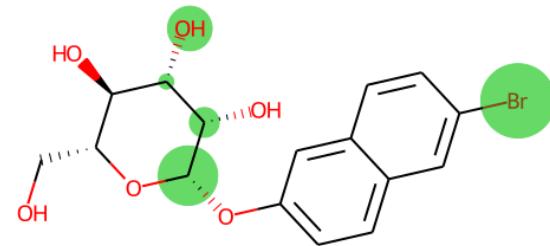
Predicted classes: N-acylpiperidine organobromine compound bromine molecular entity



SMILES: [H]C([H])(Br)Br

Atoms: CBrBr

Predicted classes: one-carbon compound organobromine compound bromine molecular entity

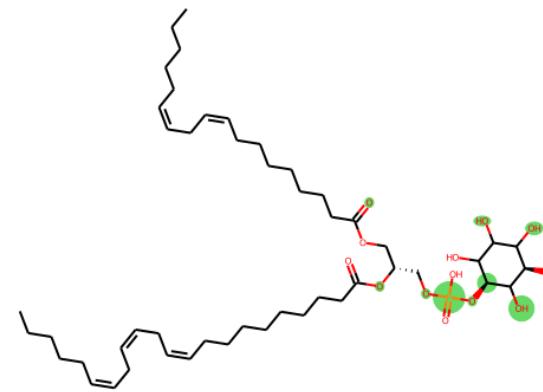


[C@H]
1.0
[C@H]
(
[C@H]
(
O
)
[C@H]
(
O
)
O
1.0
)
C
O
)
O
)
O
C
= 2.0
C
= 3.0
C
= 3.0
C
C
= 2.0
C
Br

SMILES: [C@@H]1([C@H]([C@@H](O)[C@H]([C@H](O1)CO)O)OC=2C=CC=3C=C(C=CC3C2)Br

Atoms: CCCOCCOCOOOCCCCCCCCBr

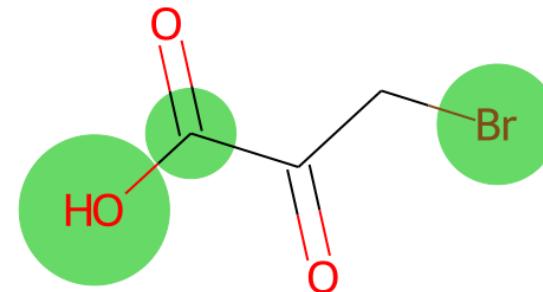
Predicted classes: organobromine compound ✕ bromine molecular entity ✕



(C@H)CC[C@H]1OCC(O)C(C)(C)C1O

SMILES: [C@H]1[C(C(C([C@H](C1O)O)O)O)OP(OC[C@H]1)(COCC(CCCCCCCC/C=C\VC/C=C\CCCCC)=O)(OC(CCCCCCCCC/C=C\VC/C=C\VC/C=C\CCCCC)=O)[H])O=O

Predicted classes: phosphatidylinositol glycerophosphoinositol

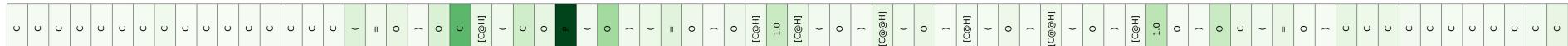
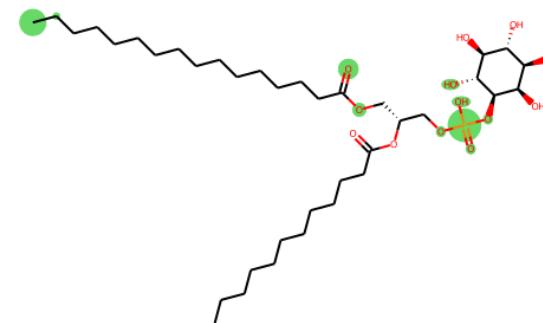


SMILES: C(O)(C(=O)CBr)=O

Atoms: COCOCBrO

Predicted classes:

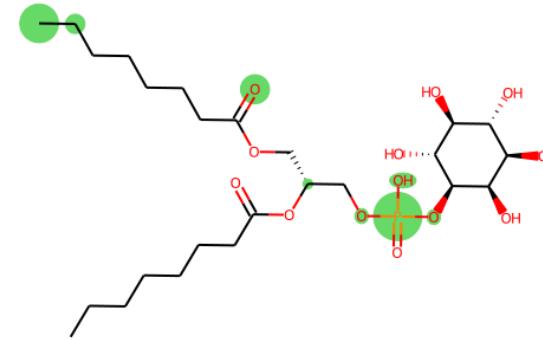
oxo monocarboxylic acid ✖organobromine compound ✖bromine molecular entity ✖oxo carboxylic acid ✖



SMILES: CCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])[C@H]1[C@H](O)[C@@H](O)[C@H](O)[C@H]1O)OC(=O)CCCCCCCCCCC

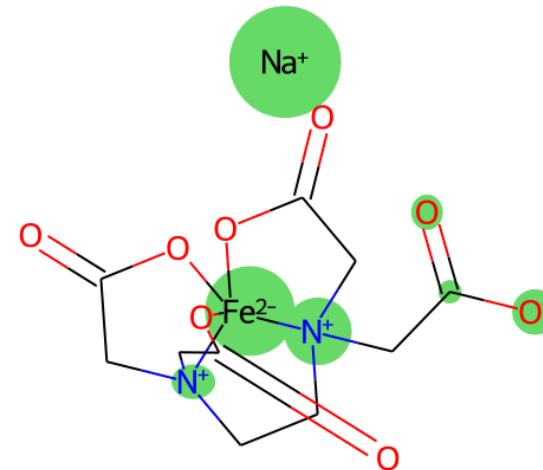
Atoms: CCCCCCCCCCCCCCOCCCCOPOOCCOCOCOCOCOCOCOCOC

Predicted classes: phosphatidylinositol ✕ glycerophosphoinositol ✕ fatty acid ester ✕



SMILES: CCCCCCCC(=O)OC[C@H](COP(=O)([O-])O[C@H]1[C@H](O)[C@@H](O)[C@H](O)[C@H](O)[C@H](O)[C@H]1O)OC(=O)CCCCCCC

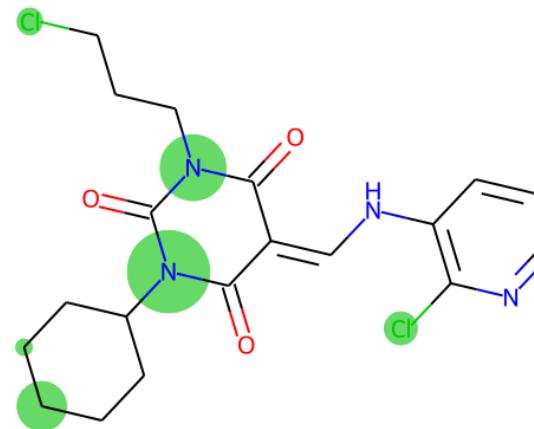
Predicted classes: phosphatidylinositol glycerophosphoinositol fatty acid ester



SMILES: [Na+].[O-]C(=O)C[N+]12CC[N+]34CC(=O)O[Fe--]13(OC(=O)C2)OC(=O)C

Atoms: NaOCOCNCCCNCCOOFeOCOCOCOC

molecular entity  iron group molecular entity  organic sodium salt  sodium salt  sodium molecular entity  alkali metal salt  transition element coordination entity  alkali metal molecular entity  coordination entity  d-block molecular entity

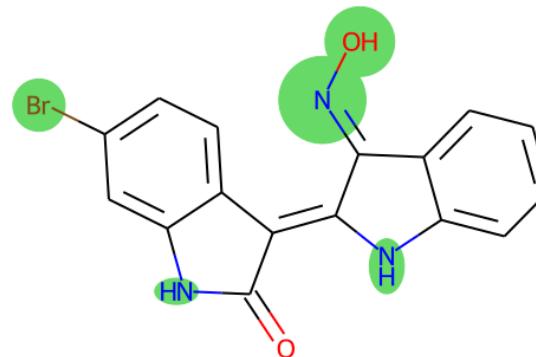


C 1.0 C C (C C) 1.0) N 2.0 C (= O) C (= CN C 3 = C (N = CC = C 3 Cl) C (= O) N (C 2 = O) C C C I
C 3.0 = C C (N) = C C 3.0) C Cl (= O)) C C (= O) C Cl

SMILES: C1CCC(CC1)N2C(=O)C(=CN=C3=C(N=CC=C3)Cl)C(=O)N(C2=O)CCCCI

Atoms: CCCCCCNCOCCNCCNC(=O)CONCOCCCCI

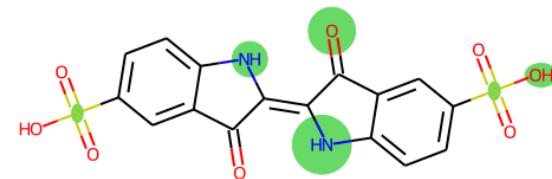
Predicted classes: barbiturates ✕ pyrimidone ✕



SMILES: O\N=C1C(\Nc2ccccc2)=C1C(=O)Nc2cc(Br)ccc2

Atoms: ONCCNCCCCCCCNC(=O)CBrCCC

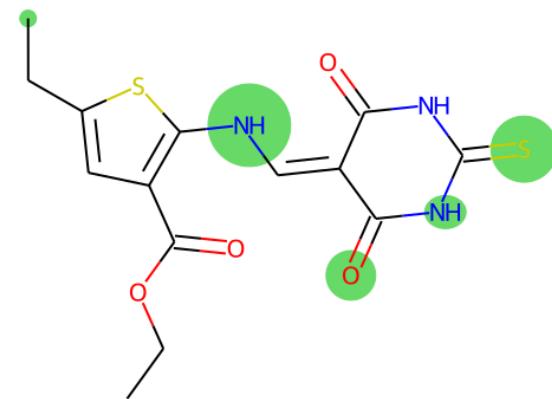
Predicted classes: gamma-lactam organobromine compound bromine molecular entity



SMILES: C=1(C=CC2=C(C1)C(NC(=C\3/NC=4C=CC(=CC4C3=O)S(O)(=O)=O)N2)=O)S(O)(=O)=O

Atoms: CCCCCCCCCNCCCCCCCOSOOONOSOOO

Predicted classes: arenesulfonic acid organosulfonic acid

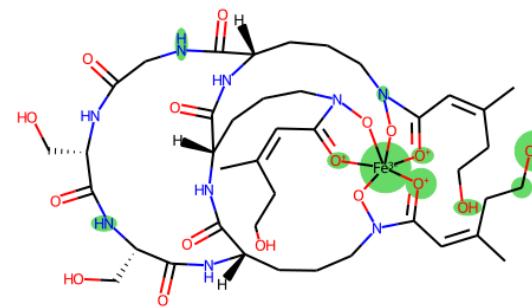


c	c	c	c	10	=	c	c	(=	c	(s	10)	n	c	=	c	2.0	c	(=	o)	z	c	(=	s)	n	c	=	o)	c	(=	o)	o	c	(=	o)	c	c
---	---	---	---	----	---	---	---	---	---	---	---	---	----	---	---	---	---	---	-----	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---

SMILES: CCC1=CC(=C(S1)NC=C2C(=O)NC(=S)NC2=O)C(=O)OCC

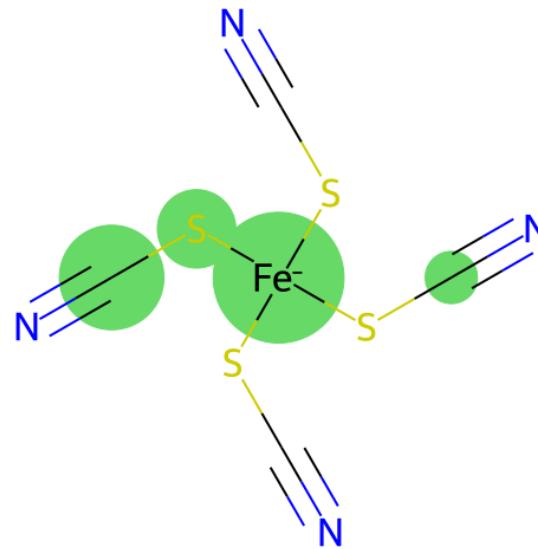
Atoms: CCCCCSNCCCONCSNCOCOCC

Predicted classes: barbiturates ✘ pyrimidone ✘



predicted
classes:

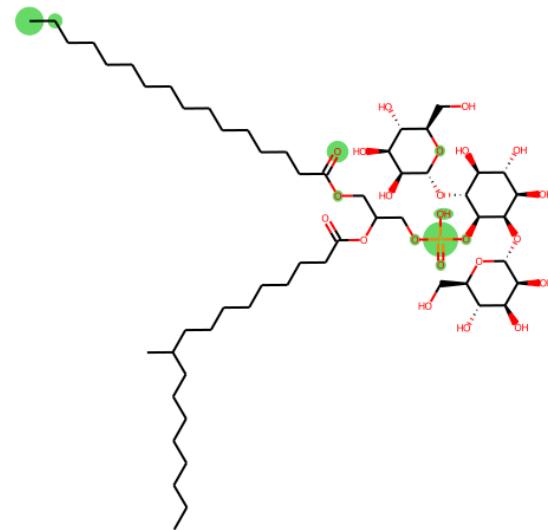
- X aliphatic alcohol
- X iron coordination entity
- X iron molecular entity
- X iron group molecular entity
- X cyclic peptide
- X transition element coordination entity
- X coordination entity
- X d-block molecular entity
- X transition element molecular entity



SMILES: N#CS[Fe-](SC#N)(SC#N)SC#N

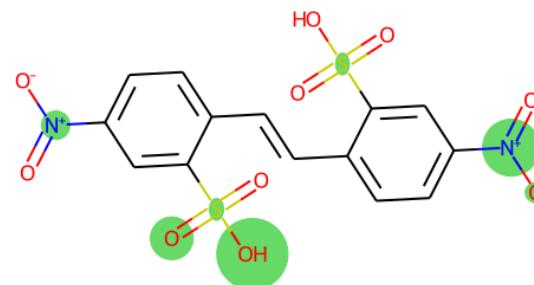
Atoms: NCSFeSCNSCNSCN

Predicted classes: iron coordination entity ✘ iron molecular entity ✘ iron group molecular entity ✘ transition element coordination entity ✘ coordination entity ✘ d-block molecular entity ✘ transition element molecular entity ✘



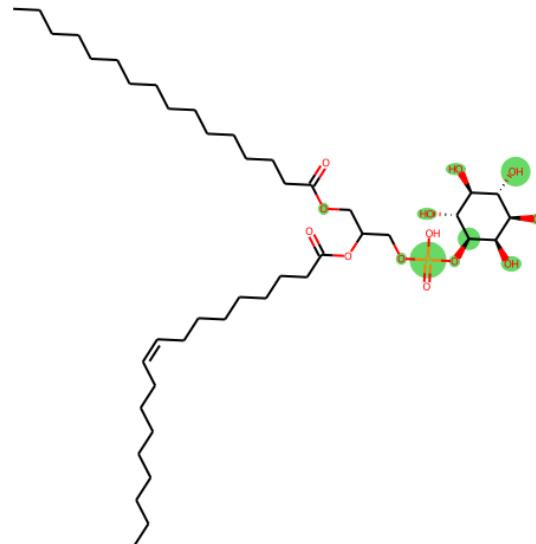
SMILES: CCCCCCCCCCCCCCCC(=O)OCC(COP(=O)([O-])C@H1C@H([O]C@H2O)C@H([CO])[C@H](O)[C@H2O)C@H([O])[C@H](O)[C@H1O)C@H([CO])[C@H](O)[C@H1O)C@H([CO])[C@H](O)[C@H1O)OC(=O)CCCCCCCCCCC(C)CCCCCCCC

Predicted classes: glycoglycerolipid glycophosholipid phosphatidylinositol glycerophosphoinositol



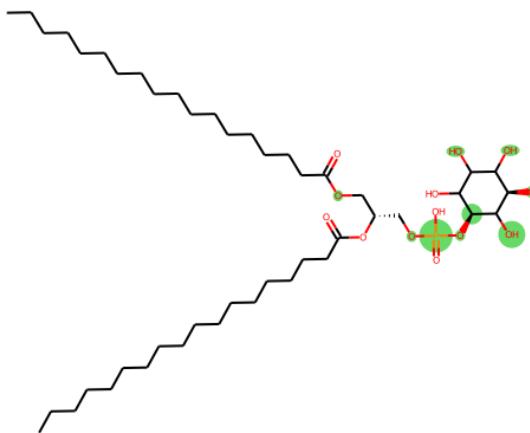
SMILES: OS(=O)(=O)c1cc(ccc1C=C\c1ccc(cc1S(O)(=O)=O)[N+](O-)=O)[N+](O-)=O
Atoms: OSOCCCCCCCCCCCCCSOOONONOONOO

Predicted classes: arenesulfonic acid organosulfonic acid



SMILES: [C@H]1([C@H]([C@H]([C@H](O)[C@H]([C@H]1O)O)O)OP(OCC(COC(=O)CCCCCCCCCCCCCCC)OC(=O)CCCCCC/C=CCCCCCCCC)(O)=O

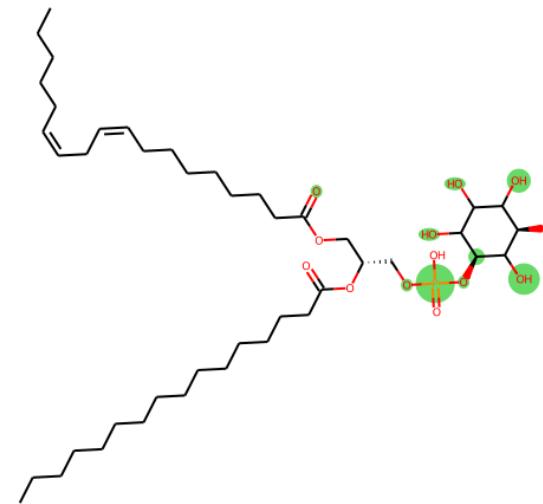
Predicted classes: phosphatidylinositol glycerophosphoinositol



SMILES: [C@@H]1(C(C([C@H](C1O)O)O)OP(OC[C@H]([COC(CCCCCCCCCCCCCC)=O](OC(CCCCCC=O)[H])O)=O

Atoms: CCCCCCOOOOOPOCCCOCCCCCCCCCCCCCOOCCCCCCCCCCCCCCOO

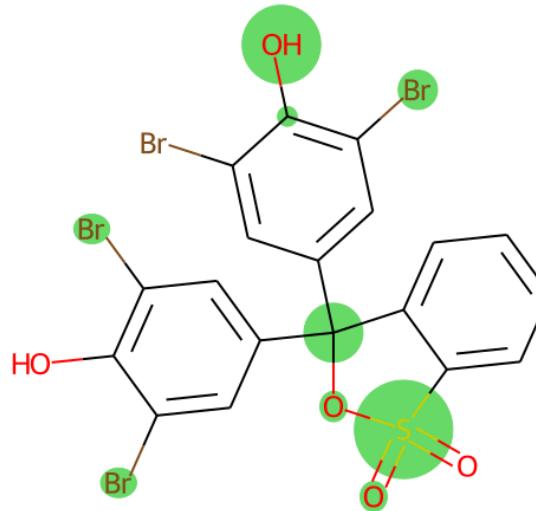
Predicted classes: phosphatidylinositol glycerophosphoinositol



SMILES: [C@H]1(C(C(C([C@H](C1O)O)O)O)OP(OC[C@H]2(COC(CCCCCCCC/C=C\C/C=C\CCCCC)=O)(OC(CCCCCCCCCCCCCCCC)=O)[H])O)=O

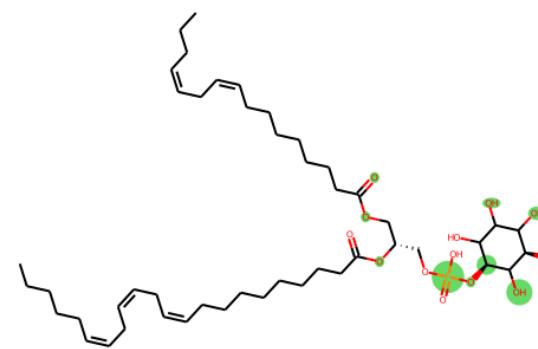
Atoms: CCCCCCOOOOOOPOCCCOCCCCCCCCCCCCCCCCCOOCCCCCCCCCCCCCCCCCCOOC

Predicted classes: phosphatidylinositol glycerophosphoinositol



SMILES: Oc1c(Br)cc(cc1Br)C1(OS(=O)(=O)c2ccccc12)c1cc(Br)c(O)c(Br)c1
Atoms: OCCBrCCCCBrCOSOOCCCCCCBrCOCBrC

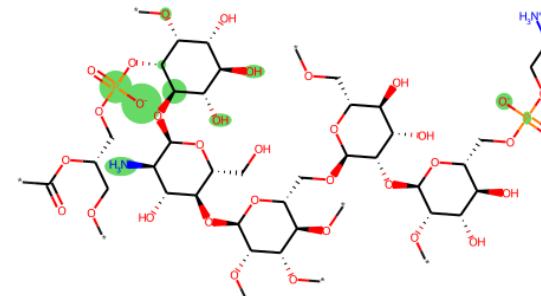
Predicted classes: organobromine compound bromine molecular entity



SMILES: [C@H]1[C(C(C([C@H](C1O)O)O)OP(OC[C@H](COC(CCCCCC/C=C/C/C=C/C=O)OC(CCCCCCCC/C=C/C/C=C/C=O)[H])O)=O

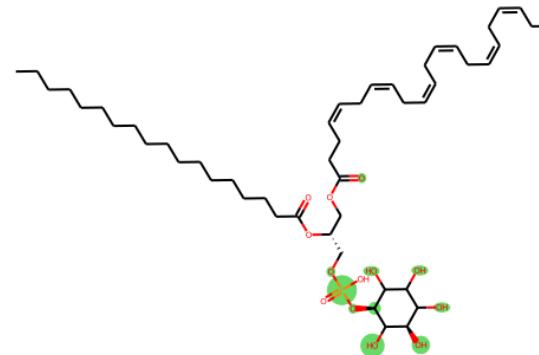
Atoms: CCCCCCOOOOOPOCCCCCCCCCCCOCCCCCCCCCCCCCCCCCCCCCOOO

Predicted classes: phosphatidylinositol ✕ glycerophosphoinositol ✕

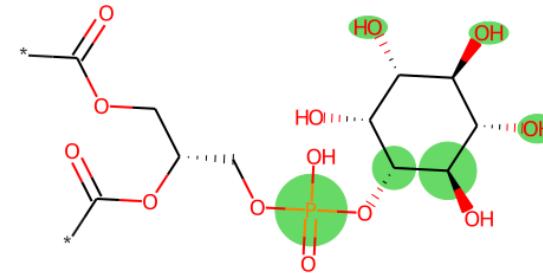


Atoms: CCCCCCOC(=O)O*OP(=O)([O-])OC(=O)*OCCN(C)COC(=O)OCCCCCOC(=O)CCCCCOC(=O)*OOC(=O)COCOP(=O)([O-])OC(=O)OCCN(=O)O*

Predicted classes: glycoglycerolipid glycoprophospholipid phosphatidylinositol glycerophosphoinositol



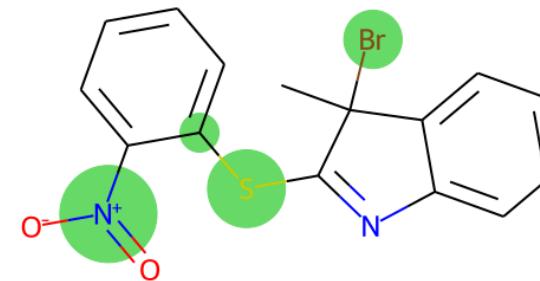
Predicted classes: phosphatidylinositol glycerophosphoinositol



SMILES: [C@H]1[C@H]([C@H]([C@H]([C@H]([C@H]([C@H]1O)O)O)O)OP(OC[C@H](COC(*)=O)OC(=O)*)=(=O)O)C

Atoms: CCCCCCOOOOPOCCOC*OOCO*OOC

Predicted classes: phosphatidylinositol glycerophosphoinositol



SMILES: CC1(Br)C(Sc2ccccc2[N+](O-)=O)=Nc2ccccc1

Atoms: CCBrCSCCCCCCNOONCCCCC

Predicted class

aryl sulfide

organobromine compound

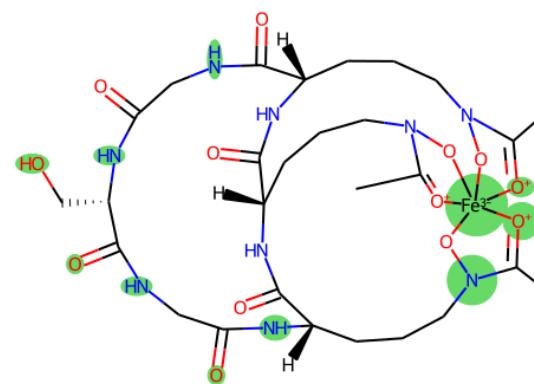
bromine molecular entity

organic sulfide

C-nitro C

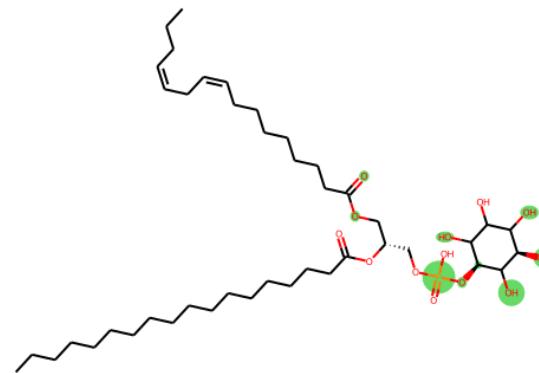
compound

nitro compound



SMILES: CC1=[O+][Fe-3]2345ON1CCC[C@H]1NC(=O)CNC(=O)[C@H](CO)NC(=O)CNC(=O)[C@H](CCCN(O2)C(C)=O+3)NC(=O)[C@H](CCCN(O4)C(C)=O+5)NC1=O
 Atoms: CCOFeONCCCCNCOCNCOCOCOCNCOCOCOCNOCCNOCOCOCNOCCNOC

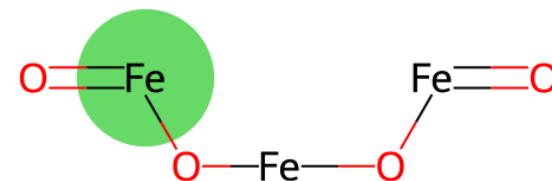
Predicted classes: iron coordination entity ✕ iron molecular entity ✕ iron group molecular entity ✕ cyclic peptide ✕ transition element coordination entity ✕ coordination entity ✕ d-block molecular entity ✕ transition element molecular entity ✕



SMILES: [C@@H]1(C(C([C@H](C1O)O)O)OP(OC[C@H](COC(CCCCCCCC/C=C/C=C\CCCC)=O)(OC(CCCCCCCCCCCCCCCCC)=O)[H])O=O

Atoms: CCCCCCOOOOOOPOCCCCOCCCCCCCCCCCCCOOCCCCCCCCCCCCCCCCCOO

Predicted classes: phosphatidylinositol ✕ glycerophosphoinositil ✕

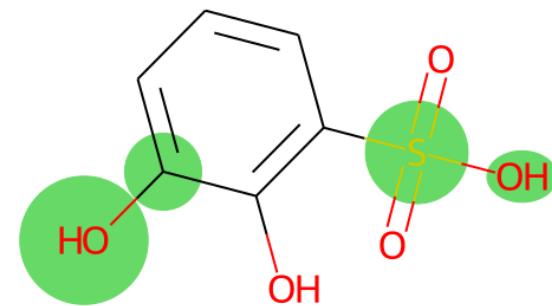


SMILES: O=[Fe]O[Fe]O[Fe]=O

Atoms: OFeOFeOFeO

Predicted classes:

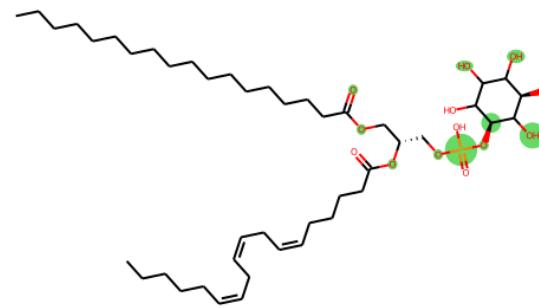
iron molecular entity iron group molecular entity d-block molecular entity transition element molecular entity



SMILES: Oc1cccc(c1O)S(O)(=O)=O

Atoms: OCCCCCCOSOOO

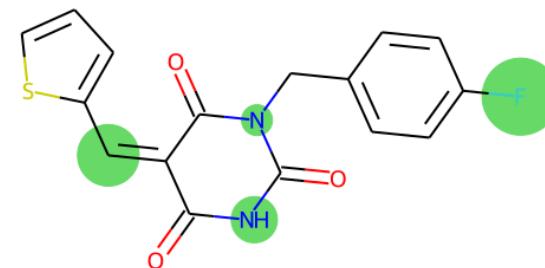
Predicted classes: arenesulfonic acid organosulfonic acid catechols benzenediols



SMILES: [C@ @H]1(C(C(C([C@H](C1O)O)O)OP(OC[C@ @](COCC(CCCCCC)C=O)(OC(CCCC/C=C\C/C=C\CCCC)=O)[H])(O)=O

Atoms: CCCCCCOOOOOPOCCCCCCCCCCCCCCCCCOOCCCCCCCCCCCCCCOO

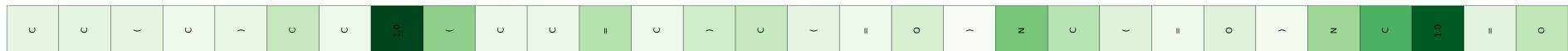
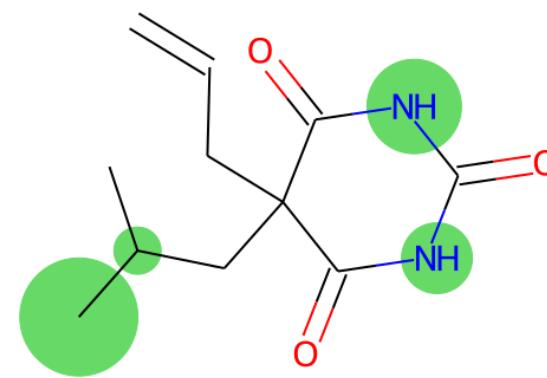
Predicted classes: phosphatidylinositol glycerophosphoinositol



SMILES: C1=CSC(=C1)C=C2C(=O)NC(=O)N(C2=O)CC3=CC=C(C=C3)F

Atoms: CCSCCCCCONCONCOCCCCCCCFC

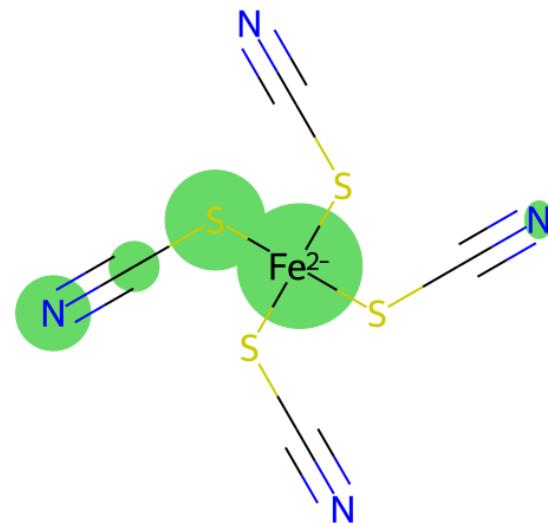
Predicted classes: barbiturates ✘ pyrimidone ✘



SMILES: CC(C)CC1(CC=C)C(=O)NC(=O)NC1=O

Atoms: CCCCCCCCNONCONCO

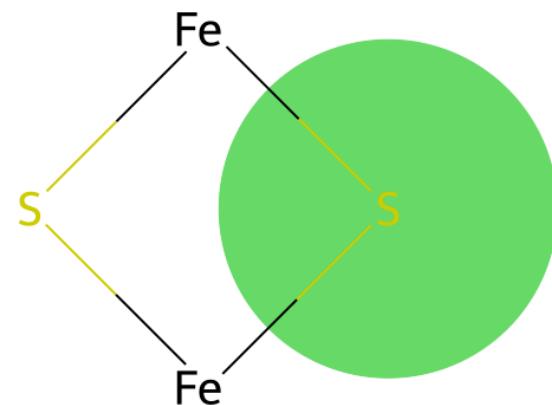
Predicted classes: barbiturates ✘ pyrimidone ✘



SMILES: N#CS[Fe--](SC#N)(SC#N)SC#N

Atoms: NCSFeSCNSCNSCN

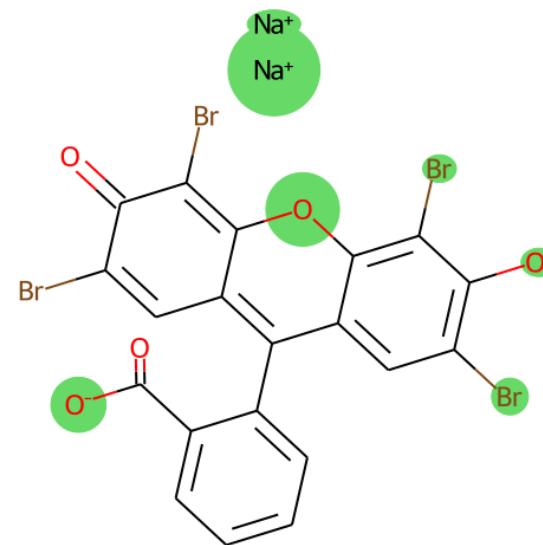
Predicted classes: iron coordination entity ✘ iron molecular entity ✘ iron group molecular entity ✘ transition element coordination entity ✘ coordination entity ✘ d-block molecular entity ✘ transition element molecular entity ✘



SMILES: S1[Fe]S[Fe]1

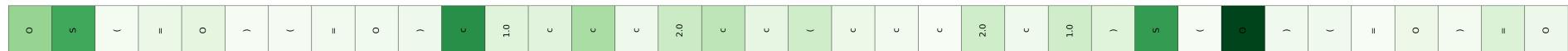
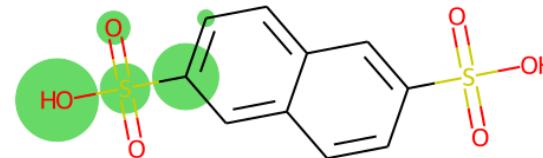
Atoms: SFeSFe

Predicted classes: iron coordination entity ✘ iron molecular entity ✘ iron group molecular entity ✘ transition element coordination entity ✘ coordination entity ✘ d-block molecular entity ✘ transition element molecular entity ✘



[Na+] . [Na+] . [O-] C (= O) c1ccccc1 - c1c2cc(Br)c([O-])c(Br)c2oc2c(Br)c(=O)c(Br)cc12
Atoms: NaNaOOCOCBrCOBrCOCCBrCOCBrCC

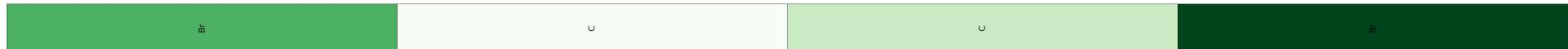
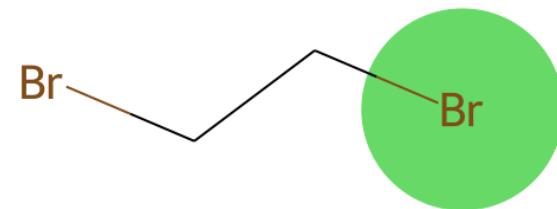
Predicted classes: organobromine compound ✗ organic sodium salt ✗ sodium salt ✗ sodium molecular entity ✗ bromine molecular entity ✗ alkali metal salt ✗ alkali metal molecular entity ✗



SMILES: OS(=O)(=O)c1ccc2cc(ccc2c1)S(O)(=O)=O

Atoms: OSOOCCCCCCCCCCSOOO

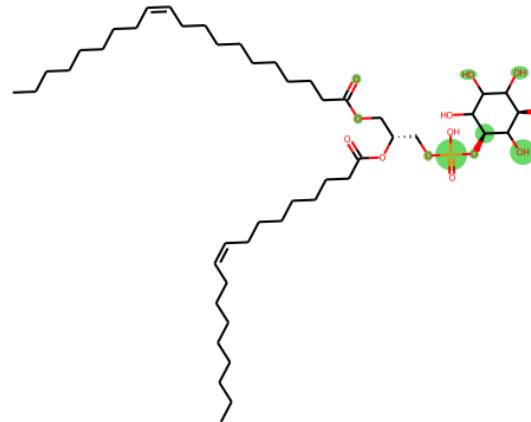
Predicted classes: arenesulfonic acid organosulfonic acid



SMILES: BrCCBr

Atoms: BrCCBr

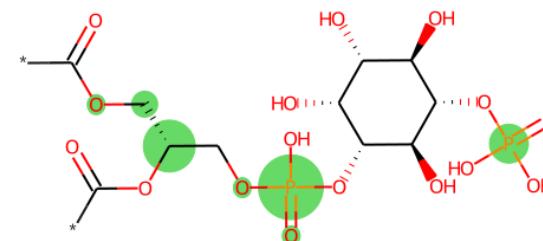
Predicted classes: organobromine compound bromine molecular entity



SMILES: [C@H]1(C(C(C([C@H](C1O)O)O)OP(OC[C@H]([COC(CCCCCC/C=C\CCCCCC)=O](OC(CCCCCC/C=C\CCCCCC)=O)[H])(O)=O

Atoms: CCCCCCOOOOOPOCCCCCCCCCCCCCCCCCCCCCOCCCCCCCCCCCCCCCCCOOO

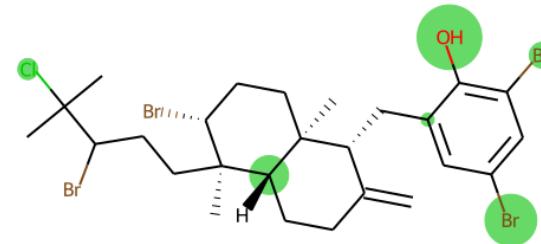
Predicted classes: phosphatidylinositol ✕ glycerophosphoinositol ✕



SMILES: [H][C@@](COC([*])=O)(COP(=O)([O])[C@H]1[C@H](O)[C@H](O)[C@H](O)[C@H](OP(=O)([O])[C@H]1O)OC([*])=O

Atoms: CCOC*OCOPOOCCOCOCOCOPOOOCOOC*O

Predicted classes: phosphatidylinositol ✕ glycerophosphoinositol ✕

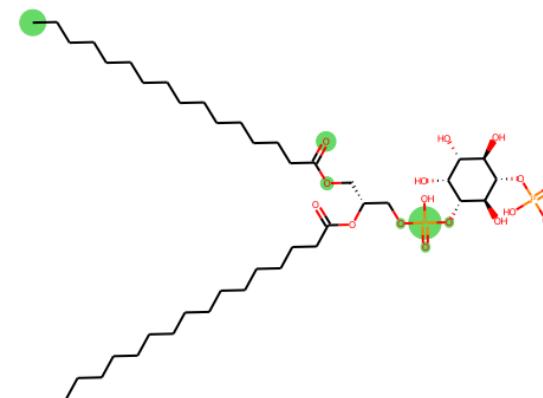


[H] [C@] 1.0
2.0
c c)
(= c)
[C@@H] ((c c ((3.0
Br)) c) (Br)) 3.0 o)
[C@] 1.0 ((c))
2.0) (c) (c)
c) (c) (c)
[C@@H] ((c))
Br)) c) (c) Cl
Cl

SMILES: [H][C@]12CCC(=C)[C@ @H](Cc3cc(Br)cc(Br)c3O)[C@]1(C)CC[C@ @H](Br)[C@]2(C)CCC(Br)C(C)(C)Cl

Atoms: CCCCCCCCCBrCCBrCOCCCCCCBrCCCCCBrCCCCI

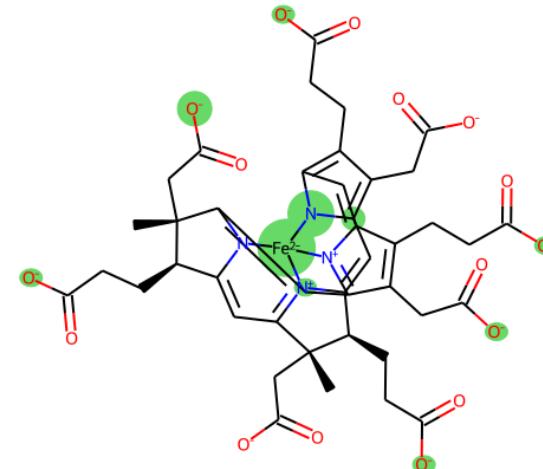
Predicted classes: organobromine compound ✕ bromine molecular entity ✕



SMILES: CCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])[C@@H]1[C@H](O)[C@H](O)[C@@H](O)[C@H](O)[OP(=O)([O-])[C@H]1O)OC(=O)CCCCCCCCCCCCCCC

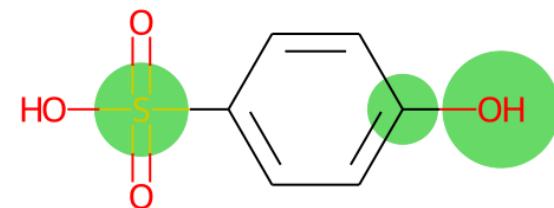
Atoms: CCCCCCCCCCCCCCCCOOC(COP(=O)([O-])[C@@H]1[C@H](O)[C@H](O)[C@@H](O)[C@H](O)[OP(=O)([O-])[C@H]1O)OC(=O)CCCCCCCCCCCCCCC

Predicted classes: phosphatidylinositol ✕ glycerophosphoinositol ✕



SMILES: C[C@]1(CC([O-])=O)[C@H](CCC([O-])=O)C2=CC3=[N+]4C(=Cc5c(CC([O-])=O)c(CCC([O-])=O)c6C=C7C(CCC([O-])=O)=C(CC([O-])=O)C8=[N+]7[Fe-]4(N2C1=C8)n56)[C@@H](CCC([O-])=O)[C@]3(C)CC([O-])=O
Atoms: CCCCOCCCCCOCCCCNCCCCCOCCCCCOCCCCCOCCCCNFeNCCNCCCCOCCCCO

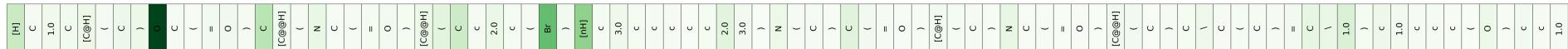
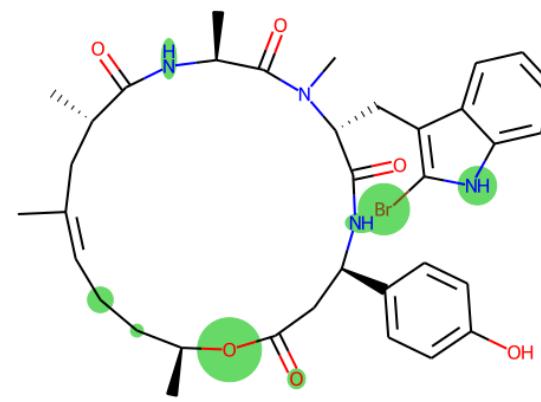
tallotetrapyrrole porphyrins iron molecular entity iron group molecular entity cyclic tetrapyrrole cyclic polypyrrole tetrapyrrole polypyrrole transition element coordination entity coordination entity d-block molecular entity



SMILES: Oc1ccc(cc1)S(=O)(=O)O

Atoms: OCCCCCCSOOO

Predicted classes: arenesulfonic acid organosulfonic acid



SMILES: [H]C1C[C@H](C)OC(=O)C[C@H](NC(=O)[C@@H](Cc2cc(Br)[nH]c3cccc23)N(C)C(=O)[C@H](C)NC(=O)[C@@H](C)C\CC(C)=C\1)c1ccc(O)cc1

Atoms: CCCCCOCOCNCOCCCCCBrNCCCCCNCCCOCCNCOCCCCCCCOCC

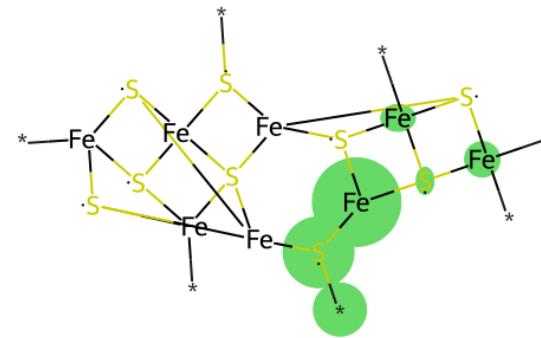
Predicted classes:

cyclodepsipeptide ✕

depsipeptide ✕

organobromine compound ✕

bromine molecular entity ✕

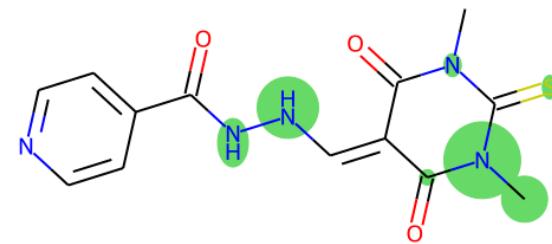


[r]	[s]	1.0	[Fe]	2.0	[s]	3.0	[Fe]	4.0	[Fe]	3.0	([r])	[s]	2.0	[Fe]	4.0	[s]	3.0	([r])	[s]	2.0	[Fe]	4.0	[s]	3.0	[Fe]	5.0	[r]	6.0	([r])	[s]	5.0	[Fe]	6.0	([r])	[s]	7.0	[Fe]	5.0	([r])	[s]	6.0
-----	-----	-----	------	-----	-----	-----	------	-----	------	-----	---	-----	---	-----	-----	------	-----	-----	-----	---	-----	---	-----	-----	------	-----	-----	-----	------	-----	-----	-----	---	-----	---	-----	-----	------	-----	---	-----	---	-----	-----	------	-----	---	-----	---	-----	-----

SMILES: [*][S]1[Fe]2[S]3[Fe](*)[*][S]4[Fe]3(*)[S]2[Fe]42[S](*)[Fe]34[S]5[Fe]6(*)[S]7[Fe]5(*)S23[Fe]17[S]46

Atoms: *SFeSFe**SFe*SFeS*FeSFe*SFe*SFeS

Predicted classes: iron coordination entity iron molecular entity iron group molecular entity transition element coordination entity coordination entity d-block molecular entity transition element molecular entity

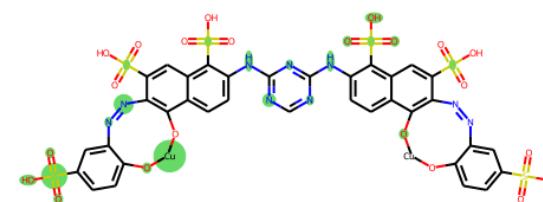


C N 1.0 C (= O)) C (= N N C (= O) C 2 = C C = N C = C 2 C (= O) N (C 1 = S) C

SMILES: CN1C(=O)C(=CN(C(=O)C2=CC=C(NC(=O)C(C=C1)N(C=C2)S(=O)(=O)C)C)C

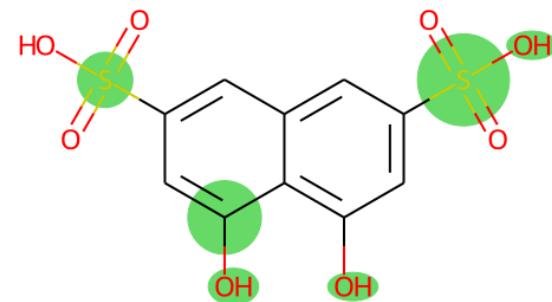
Atoms: CNCOCNNNCOCNNCCCNCCSC

Predicted classes: barbiturates ✘ pyrimidone ✘



SMILES: OS(=O)(=O)c1ccc2O[Cu]Oc3c(\N=N\c2c1)cc1c(c(Nc2ncn(C(=O)cccc6O[Cu]Oc7ccc(cc7\N=N\c6c(cc5c4S(O)(=O)=O)S(O)(=O)=O)S(O)(=O)=O)O)n2)ccc3)S(O)(=O)=O)S(O)(=O)=O)

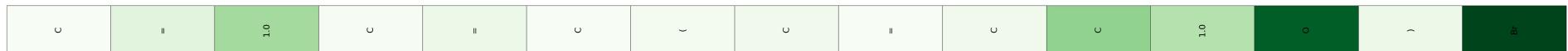
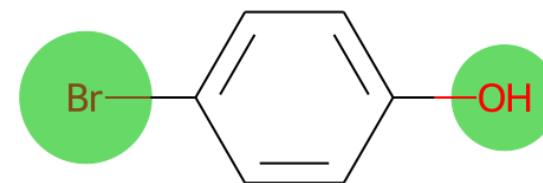
compound diamine 1,3,5-triazines arenesulfonic acid polyamine triazines azarene organosulfonic acid transition element coordination entity coordination entity d-block molecular entity transition element mole



SMILES: Oc1cc(cc2cc(cc(O)c12)S(O)(=O)=O)S(O)(=O)=O

Atoms: OCCCCCCOCOSOOOSOO

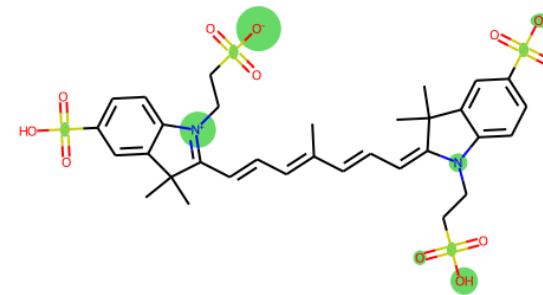
Predicted classes: hydroxynaphthalene ✘ arenesulfonic acid ✘ organosulfonic acid ✘



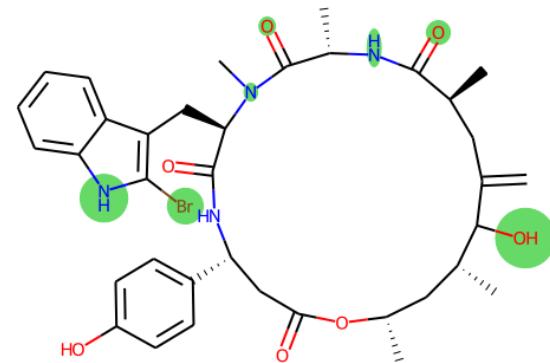
SMILES: C=1C=C(C=CC1O)Br

Atoms: CCCCCCOBr

Predicted classes: organobromine compound ✘ bromine molecular entity ✘



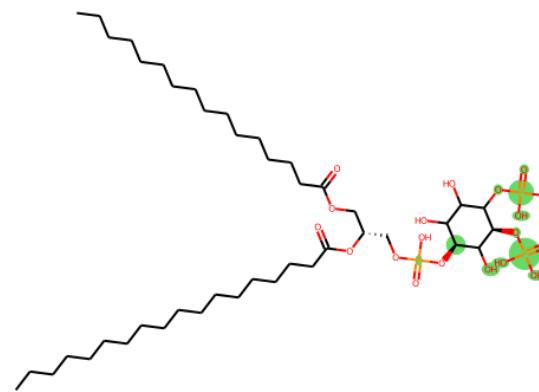
SMILES: CC(CC=C1N(CCS(=O)(=O)c2ccc(cc2C1(C)S(=O)(=O)=O)=C/C=C/C1=[N+](CCS([O-])(=O)=O)c2ccc(cc2C1(C)S(=O)(=O)=O) Atoms: CCCCCCNCCSOOOCCCCCCCCSOOOCCCCNCCSOOOCCCCCCCCSOOO Predicted classes: arenesulfonic acid organosulfonic acid



SMILES: C[C@H]1C[C@H](C)C(O)C(=C)C[C@H](C)C(=O)N[C@H](C)C(=O)N(C)[C@H](C)c2cc(Br)[nH]c3cccc23)C(=O)N[C@H](CC(=O)O1)c1ccc(O)c1

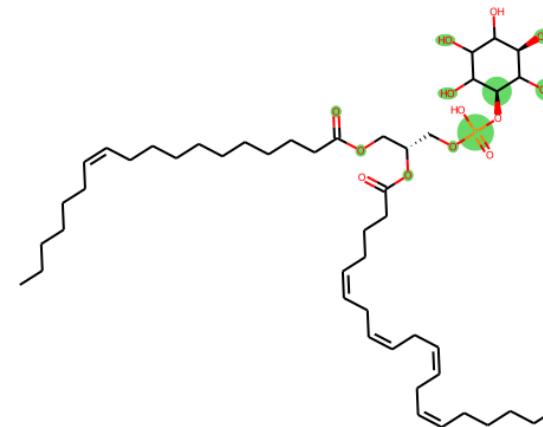
Atoms: CCCCCCOCCCCCCCONCCCONCCCCBrNCCCCCCCONCCCOOCCCCOCOC

Predicted classes: cyclodepsipeptide depsipeptide organobromine compound bromine molecular entity



SMILES: [C@H]1C(C(C([C@H](C1)OP(=O)(O)O)OP(=O)(O)O)O)OP(OC[C@H]2CCCCCCCCCCCC2)=O)(OC(CCCCCCCCCCCCCCCCC)=O)[H])(O)=O

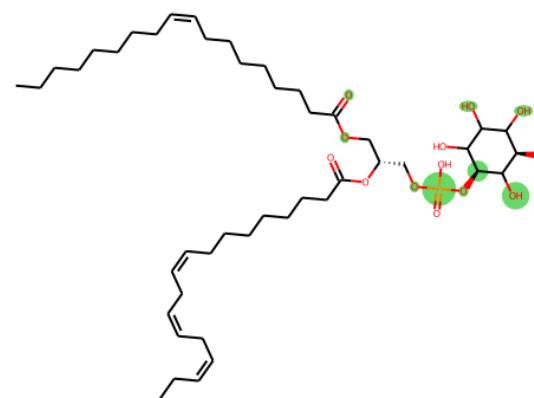
Predicted classes: phosphatidylinositol glycerophosphoinositol



SMILES: [C@H]1[C(C(C([C@H](C1O)O)O)O)OP(OC[C@H](COCCCCCCCC=C=C\CCCCCCC)=O)(OC(CCC/C=C\C/C=C\CC/C=C\CC/C=C\CCCCCCC)=O)(H)](O)=O

Atoms: CCCCCCOC(=O)OPOCCOC(=O)CCCCCCCCCCCCCCCCCCCCCOOC(=O)CCCCCCCCCCCCCCCCCCCCCOOC(=O)

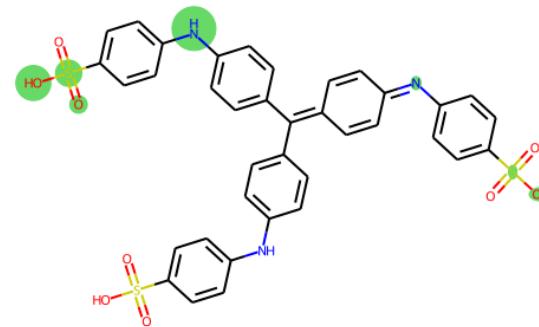
Predicted classes: phosphatidylinositol glycerophosphoinositol



SMILES: [C@@@H]1(C(C(C([C@H](C1O)O)O)O)OP(OC[C@H](COC(CCCCCCCC/C=C\CCCCCCC/C=C/C/C=C/C=C\CC)=O)(OC(CCCCCCCC/C=C/C/C=C/C=C\CC)=O)[H]))(O)=O

Atoms: CCCCCCOOOOOPOCCCOCCCCCCCCCCCCCCCCCOOCCCCCCCCCCCCCCCCCOO

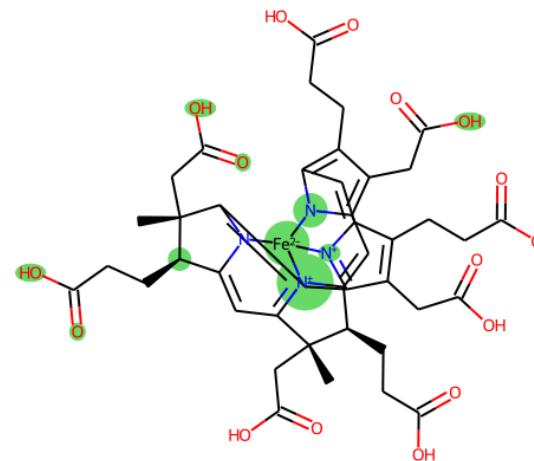
Predicted classes: phosphatidylinositol glycerophosphoinositol



SMILES: OS(=O)(=O)c1ccc(Nc2ccc(cc2)C(=C2C=CC(C=C2)=Nc2ccc(cc2)S(O)(=O)=O)c2ccc(Nc3ccc(cc3)S(O)(=O)=O)cc2)cc1

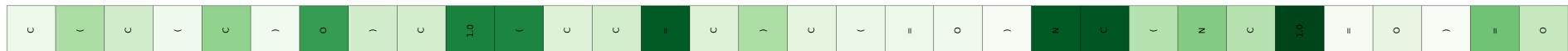
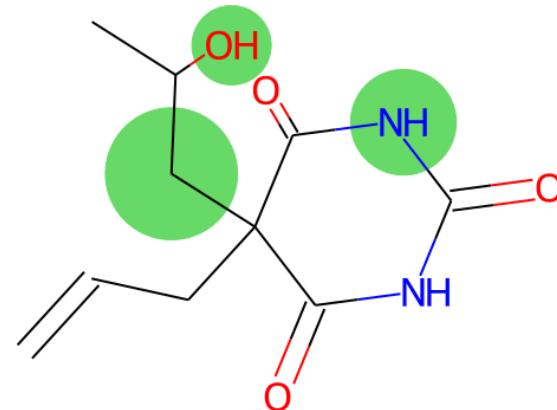
Atoms: OSOOCCCCNCCCCCCCCCCCCNCCCCCSOOOCCCCNCCCCCSOOOCCCC

Predicted classes: arenesulfonic acid organosulfonic acid secondary amino compound



Atoms: CCCCOCCCCCOOCNNCCCCCOCCCCCOCCCCCOOCNFeNCCNCCCCOCCCCO

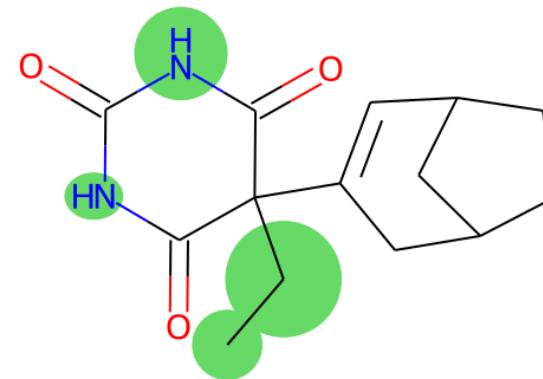
tallotetrapyrrole porphyrins iron molecular entity iron group molecular entity cyclic tetrapyrrole cyclic polypyrrole tetrapyrrole polypyrrole transition element coordination entity coordination entity d-block molecular entity



SMILES: C(C(C)O)C1(CC=C)C(=O)NC(NC1=O)=O

Atoms: CCCOCCCCCONCNO

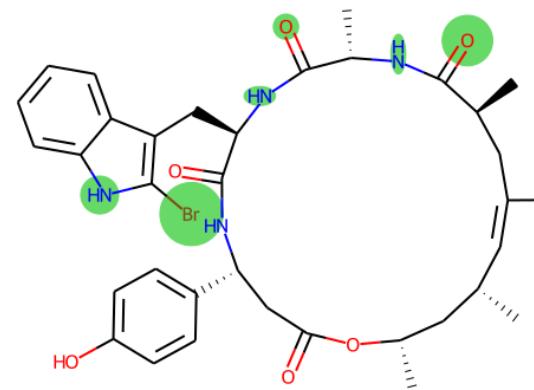
Predicted classes: barbiturates ✘ pyrimidone ✘



SMILES: C(C)C1(C(=O)NC(NC1=O)=O)C=2CC3CC(C2)CC

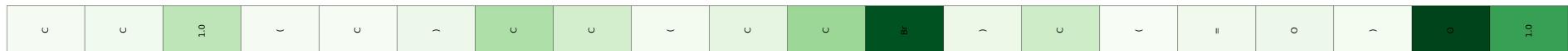
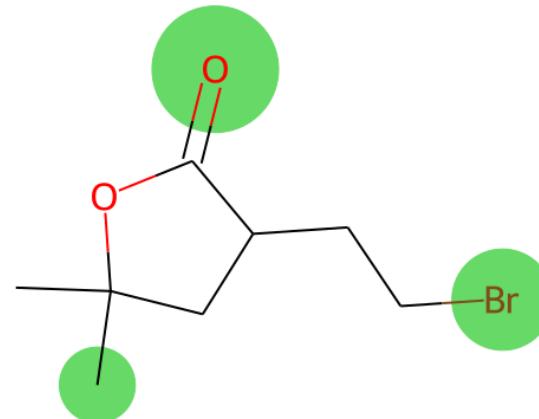
Atoms: CCCCCONCNCOOC

Predicted classes: barbiturates pyrimidone



SMILES: C[C@H]1C[C@H](C)C=C(C)C[C@H](C)C(=O)N[C@H](C)C(=O)N[C@H](Cc2c(Br)[nH]c3cccc23)C(=O)N[C@H](CC(=O)O1)c1ccc(O)cc1
Atoms: CCCCCCCCCCCCNC(=O)C(=O)N[C@H](Cc2c(Br)[nH]c3cccc23)C(=O)N[C@H](CC(=O)O1)c1ccc(O)cc1

Predicted classes: cyclodepsipeptide ✘ depsipeptide ✘ organobromine compound ✘ bromine molecular entity ✘

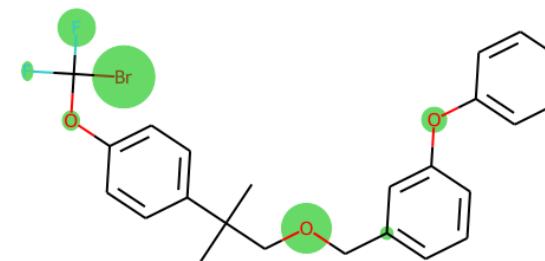


SMILES: CC1(C)CC(CBr)C(=O)O1

Atoms: CCCCCCBrCOO

Predicted classes:

organobromine compound ✖bromine molecular entity ✖oxolanes ✖gamma-lactone ✖

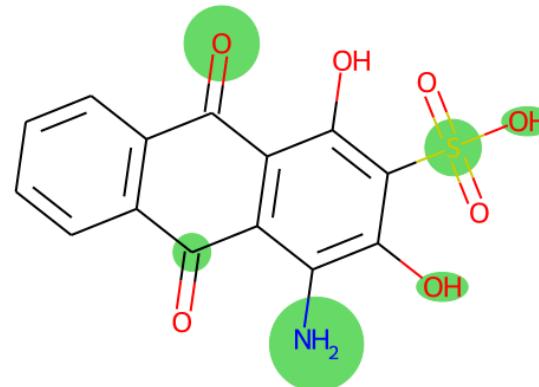


C	C	(C)	(C	O	C	c	10	C	C	C	(O	C	C	2.0	2.0)	C	C	C	C	C	C	1.0)	(O	C	C)	F	(F)))	Br)	C	C	1.0
---	---	---	---	---	---	---	---	---	---	----	---	---	---	---	---	---	---	-----	-----	---	---	---	---	---	---	---	-----	---	---	---	---	---	---	---	---	---	---	---	---	----	---	---	---	-----

SMILES: CC(C)(COCc1cccc(Oc2ccccc2)c1)c1ccc(OC(F)(F)Br)cc1

Atoms: CCCCCOCCCCCCCCOCCCCCCCCCCCCOCFFBrC

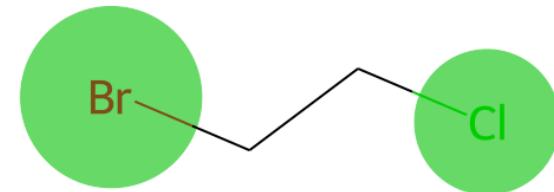
Predicted classes: organobromine compound bromine molecular entity



SMILES: C1=CC=CC2=C1C(C3=C(C2=O)C(=C(C=C3N)O)S(O)(=O)=O)O=O
Atoms: CCCCCCCCCCOCCCCNOSOOOO

dicted
sses:

- hydroxyanthraquinones X
- primary amine X
- arenesulfonic acid X
- anthraquinone X
- acenoquinone X
- organosulfonic acid X
- anthracenes X
- acenes X
- primary amino compound X
- quinone X
- carbotricyclic compound X
- amine X



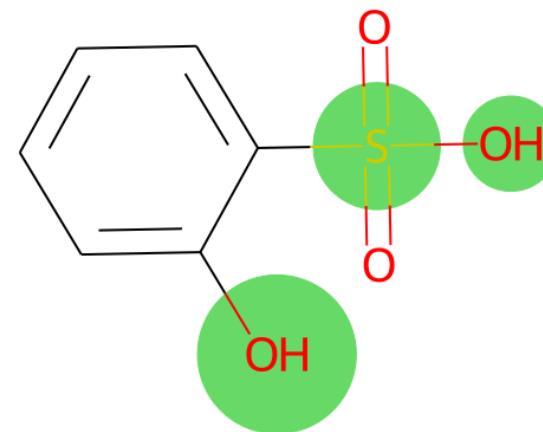
□

□

□

Br

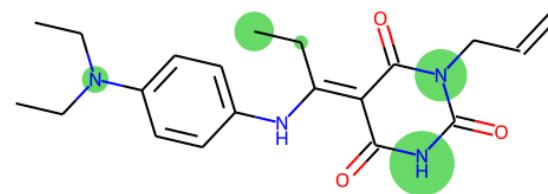
SMILES: CICCB_rAtoms: CICCB_rPredicted classes: organobromine compound bromine molecular entity



SMILES: Oc1ccccc1S(O)(=O)=O

Atoms: OCCCCCCSOOO

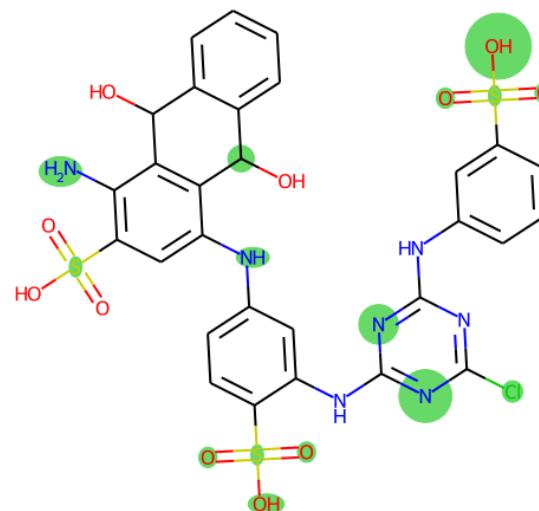
Predicted classes: arenesulfonic acid organosulfonic acid



SMILES: CCC(=C1C(=O)NC(=O)N(C1=O)CC=C)NC2=CC=C(C=C2)N(CC)CC

Atoms: CCCCCONCONCOCCCCNCCCCCNCCCC

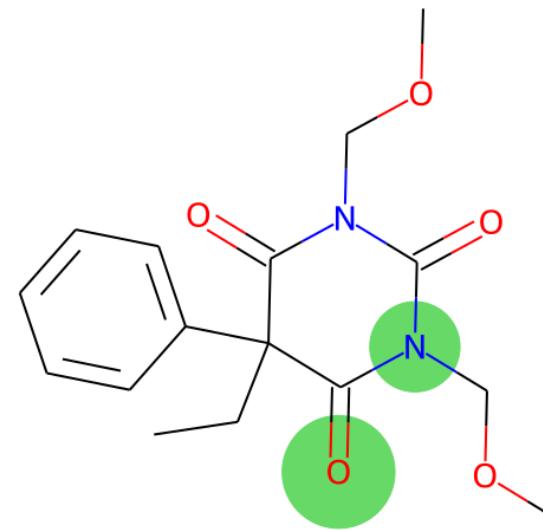
Predicted classes: barbiturates ✕ pyrimidone ✕



SMILES: Nc1c(cc(Nc2ccc(c(Nc3nc(Cl)nc(Nc4cccc(c4)S(O)(=O)=O)n3)c2)S(O)(=O)=O)c2C(O)c3cccc3C(O)c12)S(O)(=O)=O

Atoms: NCCCCNCCCCCNCCINCNCCCCCSOOONCSOOOCOCOCOCOSOO

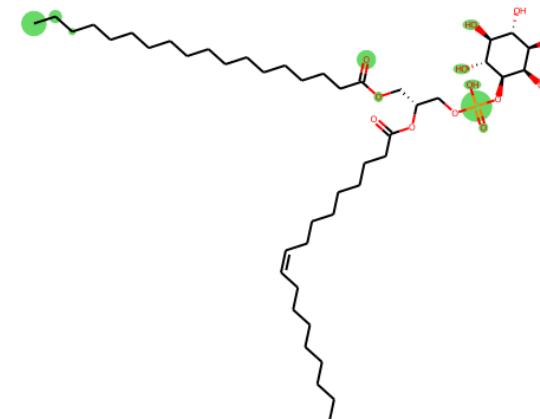
Predicted classes: diamine ✕ 1,3,5-triazines ✕ arenesulfonic acid ✕ polyamine ✕ triazines ✕ azaarene ✕ organosulfonic acid ✕ anthracenes ✕ acenes ✕ carbotricyclic compound ✕



SMILES: C(C)C1(C(=O)N(COC)C(N(C1=O)COC)=O)C2=CC=CC=C2

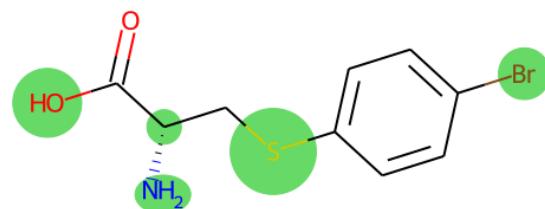
Atoms: CCCCCONCOCCNCOCOCOCOC

Predicted classes: barbiturates pyrimidone



SMILES: CCCCCCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])[C@H]1[C@H](O)[C@@H](O)[C@H]1O)[C@H](O)[C@H]1O)OC(=O)CCCCCCCC\c=C\CCCCCCCC

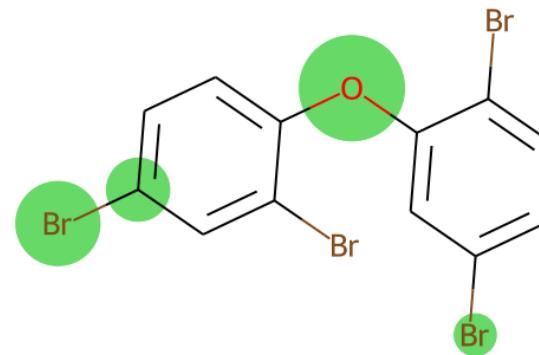
Predicted classes: phosphatidylinositol glycerophosphoinositol



SMILES: N[C@H](CSc1ccc(Br)cc1)C(=O)=O

Atoms: NCCSCCCCCBrCCCOO

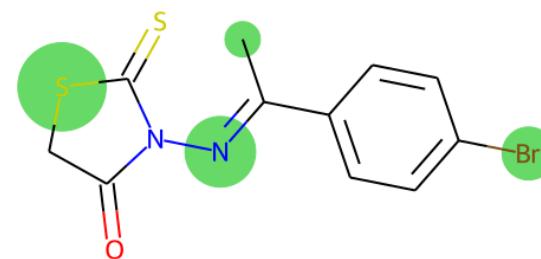
Predicted classes: sulfur-containing carboxylic acid organobromine compound bromine molecular entity organic sulfide sulfide non-proteinogenic amino acid



SMILES: Brc1ccc(Oc2cc(Br)ccc2Br)c(Br)c1

Atoms: BrCCCCOCCCBrCCCCBrCBrC

Predicted classes: organobromine compound ✖ bromine molecular entity ✖

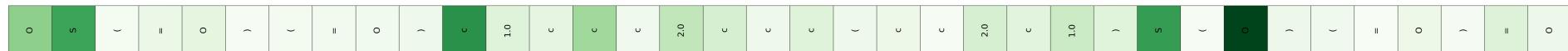
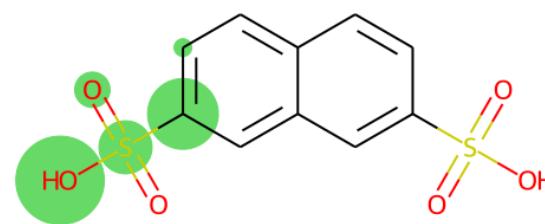


C C () = N N 1.0 C () = O) C = S C 2 = C C = C (C = C 2) Br

SMILES: CC(=NN1C(=O)CSC1=S)C2=CC=C(C=C2)Br

Atoms: CCNNCOCS SCSCCCCCBr

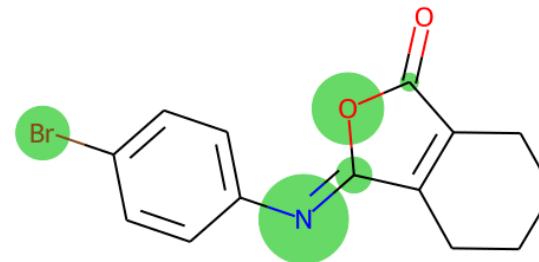
Predicted classes: organobromine compound ✕ bromine molecular entity ✕



SMILES: OS(=O)(=O)c1ccc2ccc(cc2c1)S(O)(=O)=O

Atoms: OSOOCCCCCCCCCSOO

Predicted classes: arenesulfonic acid organosulfonic acid

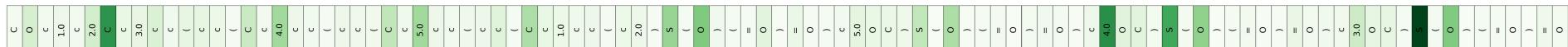
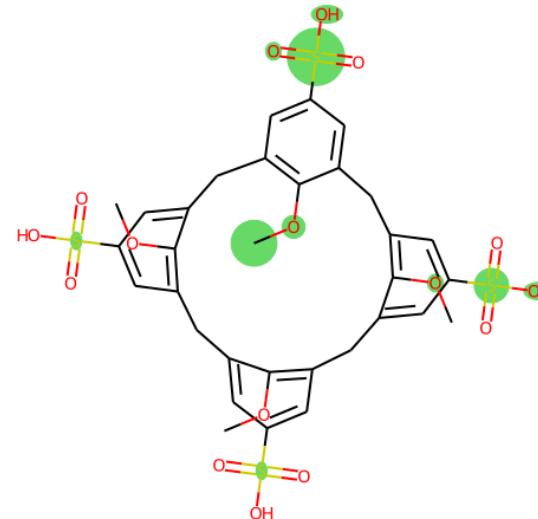


Br	c	1.0	c	c	c	(c	c	1.0)	\	n	=	c	1.0	O	c	(=	o)	c	2.0	=	c	/	1.0	c	c	c	c	2.0
----	---	-----	---	---	---	---	---	---	-----	---	---	---	---	---	-----	---	---	---	---	---	---	---	-----	---	---	---	-----	---	---	---	---	-----

SMILES: Brcccc(cc1)N=C1OC(=O)C2=C1CCCC2

Atoms: BrCCCCCNOCOCOCCCCCC

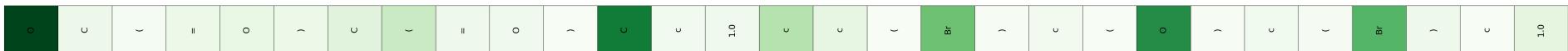
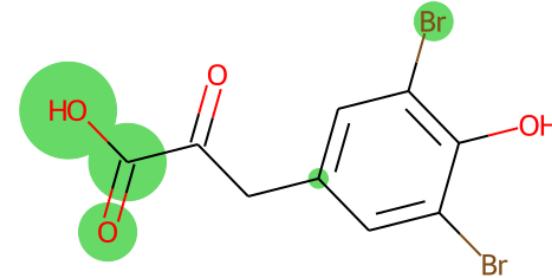
Predicted classes: organobromine compound ✕ bromine molecular entity ✕



SMILES: COc1c2Cc3cc(cc(Cc4cc(cc(Cc5cc(cc(Cc1cc(c2)S(O)(=O)=O)c5OC)S(O)(=O)=O)c4OC)S(O)(=O)=O)c3OC)S(O)(=O)=O

Atoms: COCCCCCCCCCCCCCCCCCCCCCCCCS000C0CS000C0CS000C0CS000

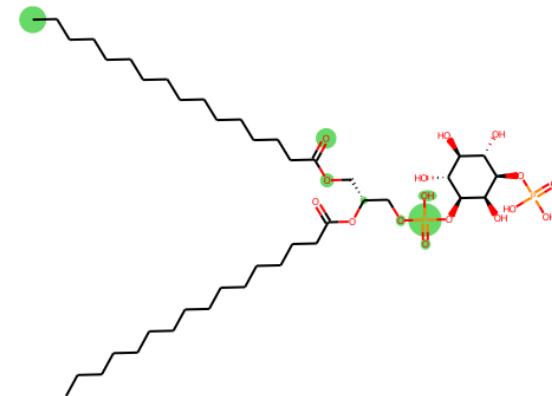
Predicted classes: arenenesulfonic acid organosulfonic acid



SMILES: OC(=O)C(=O)Cc1cc(Br)c(O)c(Br)c

Atoms: OCOCOCCCCBrCOCBr

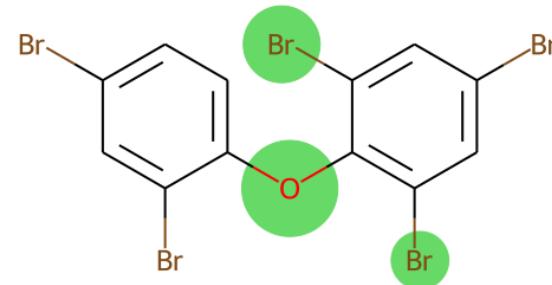
Predicted classes: oxo monocarboxylic acid organobromine compound bromine molecular entity oxo carboxylic acid



SMILES: CCCCCCCCCCCCCC(=O)OC[C@H](COP(=O)([O-])[C@H]1[C@H]1O)[C@H](O)[C@H]1O)[C@H](O)[C@H]1OP(=O)([O-])[C@H]1O)OC(=O)CCCCCCCCCCCCCCCC

Atoms: CCCCCCCCCCCCCCOOCCCOPOOOCCOCOCOCOPOOOCOOCCOC

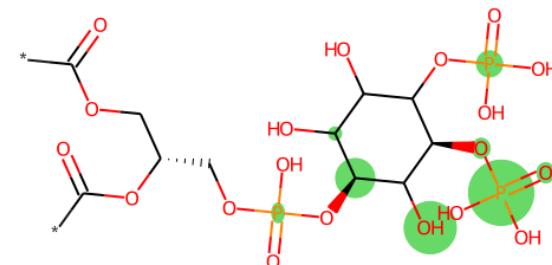
Predicted classes: phosphatidylinositol glycerophosphoinositol



SMILES: O(C=1C(=CC(=CC1Br)Br)Br)C=2C=CC(=CC2Br)Br

Atoms: OCCCCCCBrBrBrCCCCCCCBrBr

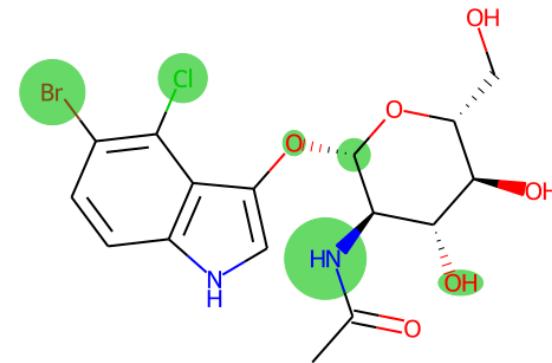
Predicted classes: organobromine compound bromine molecular entity



SMILES: [C@H]1(C(C(C([C@H](C1O)OP(=O)(O)O)OP(=O)(O)O)OP(OC[C@H](COCC(=O)OC(=O)[H])O)=O

Atoms: CCCCCCOOPOOOOPOOOOOPOCCOC*OOC*OO

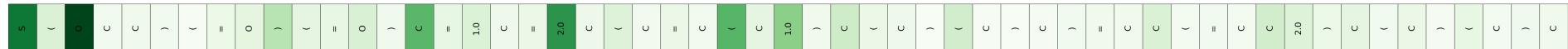
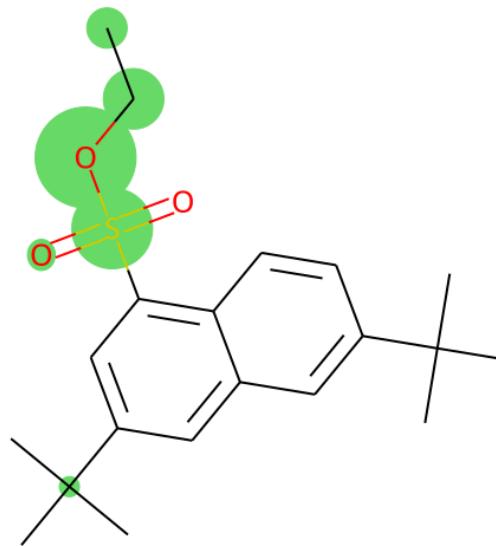
Predicted classes: phosphatidylinositol glycerophosphoinositol



SMILES: N1C=C(C2=C1C=CC(=C2Cl)Br)O[C@H]3([C@H](NC(=O)C)[C@@H](O)[C@H](O)[C@H](O3)CO)[H]

Atoms: NCCCCCCCCBrOCCNCOCCOCOCOCOC

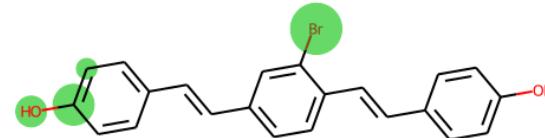
Predicted classes: amino monosaccharide organobromine compound bromine molecular entity amino sugar



SMILES: S(OCC)(=O)C=1C=2C(C=C(C1)C(C)(C)O)=CC(=CC2)C(O)(C)C

Atoms: SOCCCOCCCCCCCCCCCCCCCCCCCC

Predicted classes: arenesulfonic acid organosulfonic acid

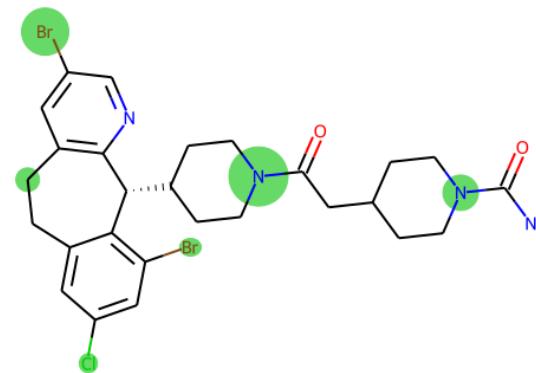


O c 1.0 c c c (\) c = C c \ / c 2.0 c c c (\) c = C c \ / c 3.0 c c c (\) O) c c c Br) c 2.0) c c 1.0

SMILES: Oc1ccc(CC=CCc2ccc(CC=Cc3ccc(O)cc3)c(Br)cc2)cc1

Atoms: OCCCCCCCCCCCCCCCCCOCCCCBrCCC

Predicted classes: organobromine compound bromine molecular entity polyphenol

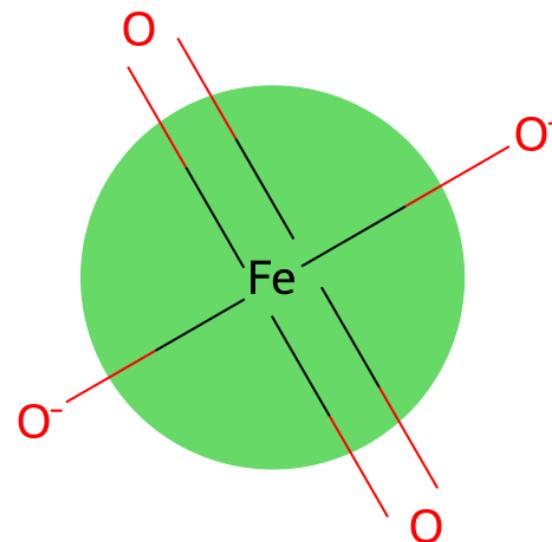


C = 1.0
C = 2.0
C
C
C
C = 3.0
C
C =
(
C
C
C = 3.0
[C@H]
(
C
C
C = 1.0
N
C
(
C
C = 2.0
Br
)
C
C
C = 4.0
C
C
C = 4.0
N
(
C
C
C = 5.0
O
)
C
C
C = 5.0
N
(
C
C
C = 6.0
N
)
C
Br
)
Cl

SMILES: C=12CCC=3C=C(C=C(C3[C@H](C1N=CC(=C2Br)C4CCN(CC4)C(=O)CC5CCN(CC5)C(N)=O)Br)Cl

Atoms: CCCCCCCCCCNCCCCBrCCCCNCCCOCCCCNCCCCNOBrCl

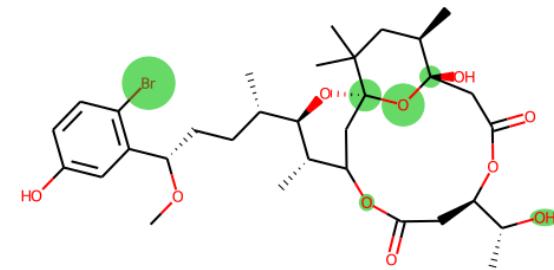
Predicted classes: N-acylpiperidine ✘ organobromine compound ✘ bromine molecular entity ✘



SMILES: [O-][Fe]([O-])(=O)=O

Atoms: OFeOOO

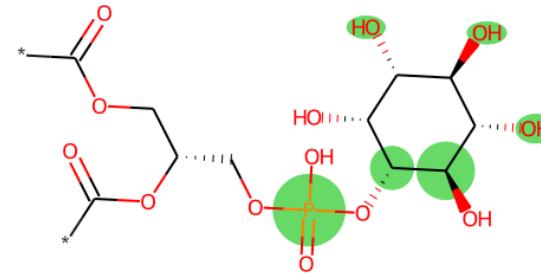
Predicted classes: iron coordination entity ✘ iron molecular entity ✘ iron group molecular entity ✘ transition element coordination entity ✘ coordination entity ✘ d-block molecular entity ✘ transition element molecular entity ✘



SMILES: [C@H]123O[C@H]([C@H](C)C1CC1(C)C)(CC1OC[C@H]1([C@H](C)O)CC1OC(C2)[C@H](C)[C@H]1O3)[C@H](C)CC[C@H](C)=C4=C(=CC=C(C4O)Br)OC1C(H)=O)[H])=O)OC

Atoms: COCCCCCCCCCOCCCCOCCOCCCCCCOCCCCCCCCCOBrOCCOO

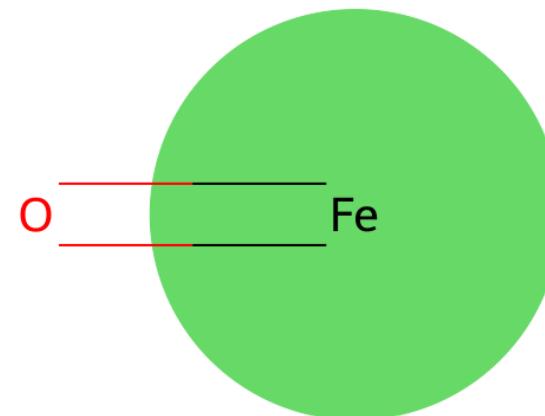
Predicted classes: ketal ✗ lactol ✗ hemiacetal ✗ oxaspiro compound ✗ acetal ✗ spiro compound ✗ organobromine compound ✗ macrolide ✗ macrocyclic lactone ✗ bromine molecular entity ✗ polyketide ✗



SMILES: [C@H]1[C@H]([C@H]([C@H]([C@H]([C@H]([C@H]1O)O)O)O)OP(OC[C@H](COC(*)=O)OC(=O)*)=(=O)O)C

Atoms: CCCCCCOOOOPOCCCOC*OOCO*OOC

Predicted classes: phosphatidylinositol glycerophosphoinositol



SMILES: O=[Fe]

Atoms: OFe

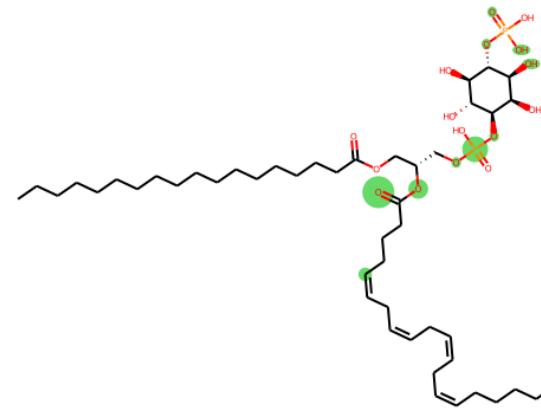
Predicted classes:

iron molecular entity

iron group molecular entity

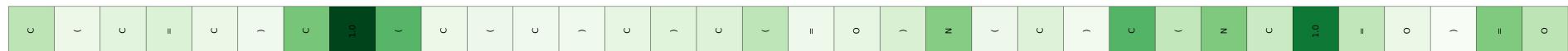
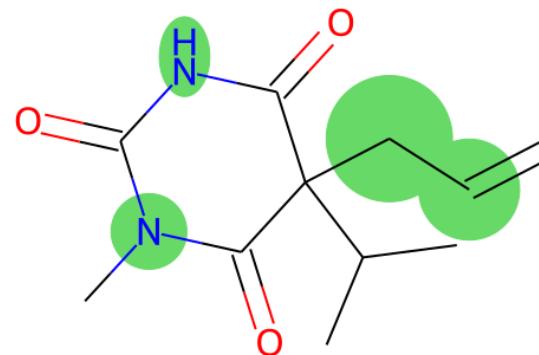
d-block molecular entity

transition element molecular entity



SMILES: O=C(CCC/C=C\C/C=C\C/C=C\C/C=CCCCCCC)O[C@H](COP(O[C@H]1C[C@H]1[C@H]1[C@H]1[C@H]1[C@H]1[C@H]1O)O)OP(O(=O)O)O)O(=O)O)COC(=O)CCCCCCCCCCCCCCCCCCCC

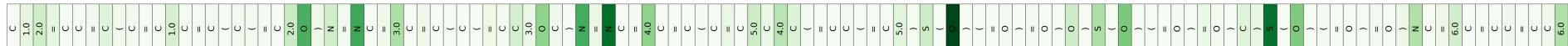
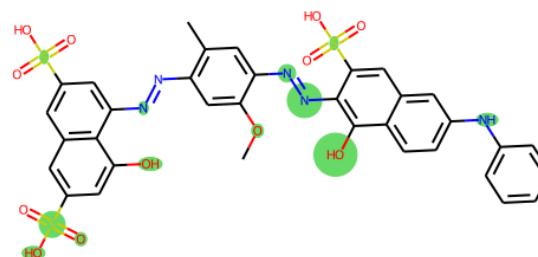
Predicted classes: phosphatidylinositol glycerophosphoinositol



SMILES: C(C=C)C1(C(C)C)C(=O)N(C)C(NC1=O)=O

Atoms: CCCCCCCCNC(=O)NCCNCO

Predicted classes: barbiturates ✘ pyrimidone ✘

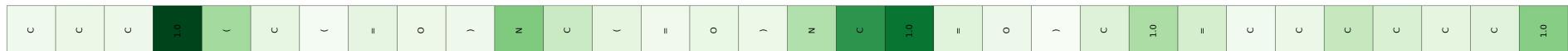
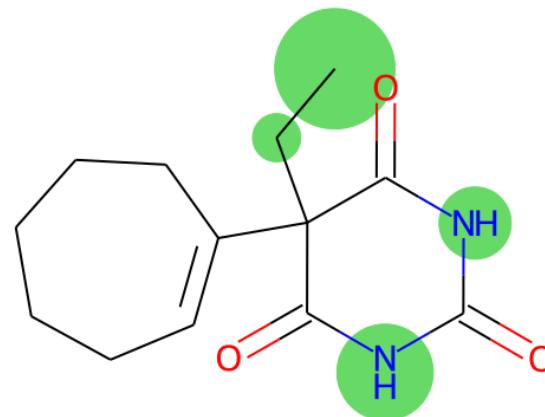


SMILES: C12=CC=C(C=C1C=C(C(=C2O)N=NC=3C=C(C(=CC3OC)N=NC=4C=C(C=C5C4C(=CC=C5)S(O)=O)=O)O)S(O)(=O)=O)C(S(O)(=O)=O)NC=6C=CC=CC6

Atoms: CCCCCCCCCCONCCCCCCCOCNNCCCCCCCSOOOSOOOCOOONCCCCC

Predicted classes:

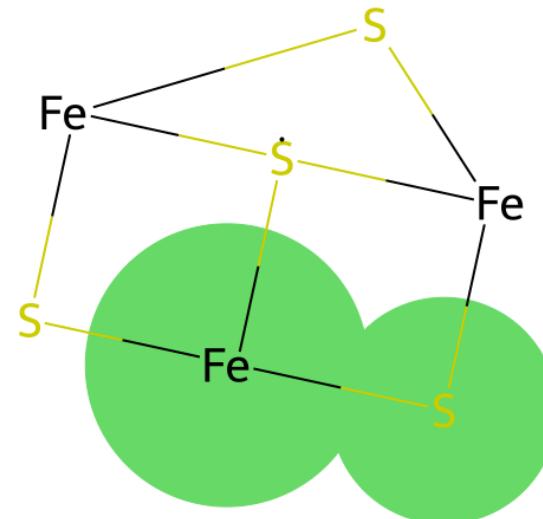
- azo compound 
- hydroxynaphthalene 
- arenesulfonic acid 
- organosulfonic acid 
- secondary amino compound 



SMILES: CCC1(C(=O)NC(=O)NC1=O)C1=CCCCCC1

Atoms: CCCCONCONCOCCCCCCC

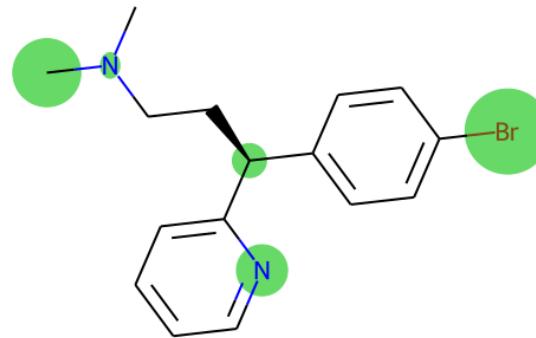
Predicted classes: barbiturates pyrimidone



SMILES: S1[Fe]2S[Fe]3S[Fe]1[S]23

Atoms: SFeSFeSFeS

Predicted classes: iron coordination entity ✘ iron molecular entity ✘ iron group molecular entity ✘ transition element coordination entity ✘ coordination entity ✘ d-block molecular entity ✘ transition element molecular entity ✘



SMILES: CN(C)CC[C@H](c1ccc(Br)cc1)c1cccn1

Atoms: CNCCCCCCCBrCCCCCN

Predicted classes: organobromine compound (X) bromine molecular entity (X)