

Getting the SMILES right: Identifying inconsistent chemical identities in the ECHA database, PubChem and the CompTox Chemicals Dashboard – Supporting Information 2

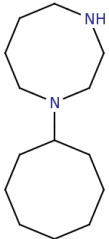
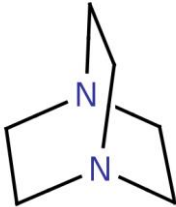
Juliane Glüge, Kristopher McNeill and Martin Scheringer

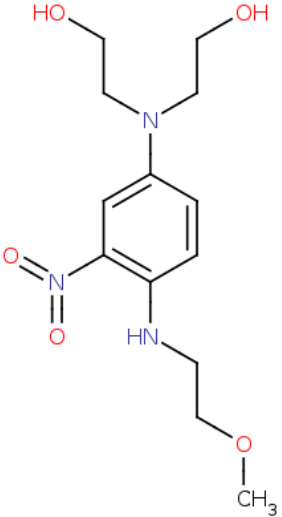
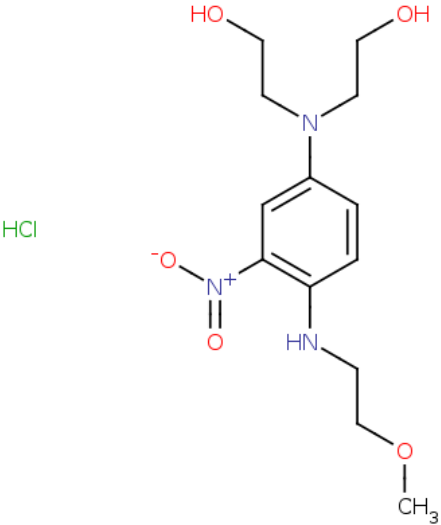
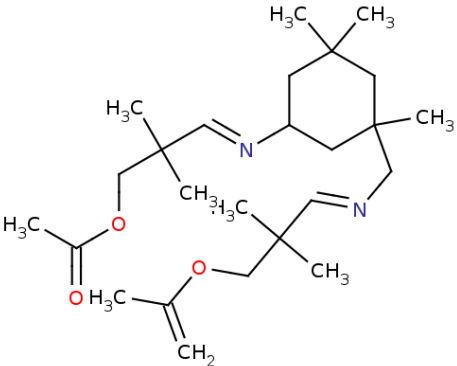
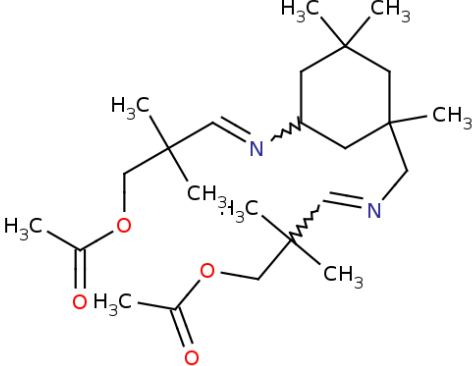
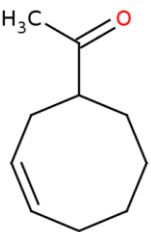
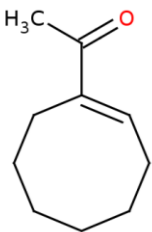
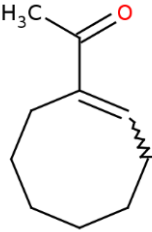
Substances in the ECHA database where the SMILES do not correspond to the Chemical Abstract Service Registry Number™ (CAS RN™) as allocated in SciFinderⁿ

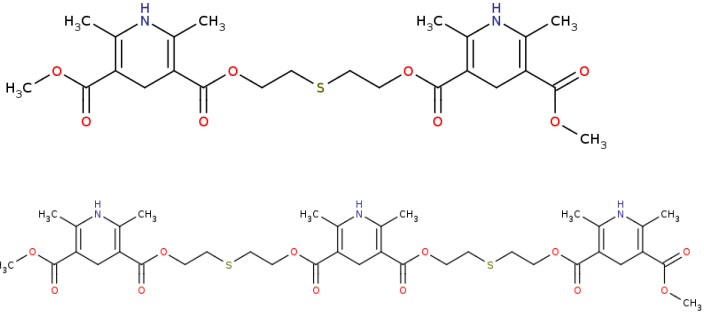
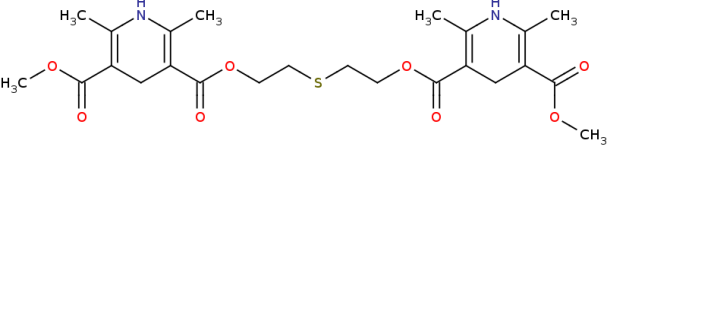
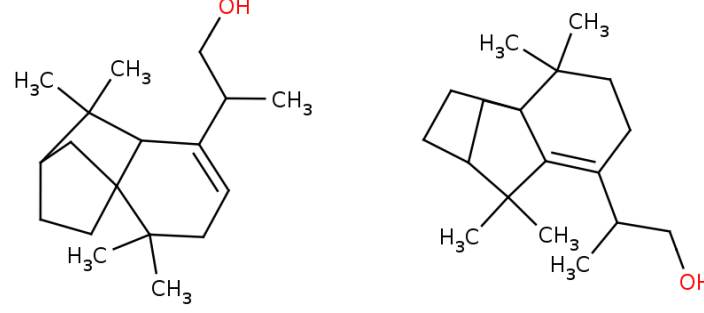
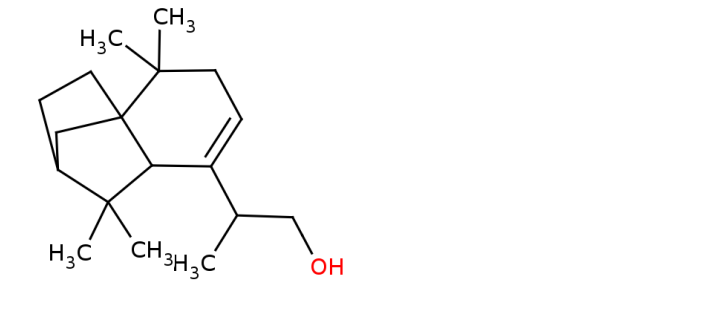
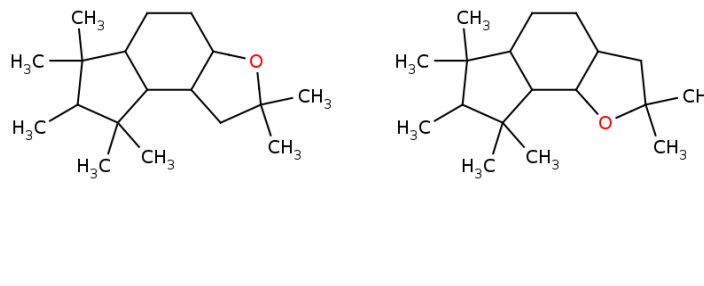
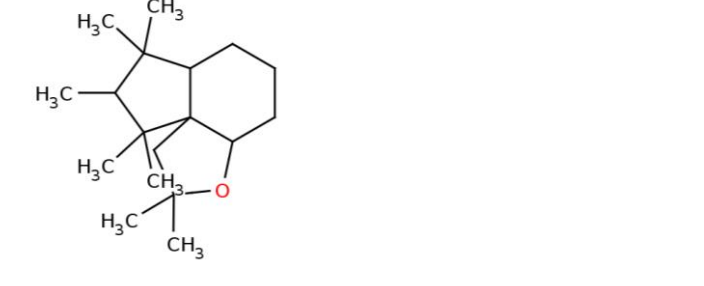
For the SMILES and names of the compounds, please refer to the Supporting Information-1 of this article. Please note that due to the large number of structures, mistakes cannot be excluded completely, and we assume no liability for the molecules shown. The information shown here correspond to the ECHA database as of January 2021.

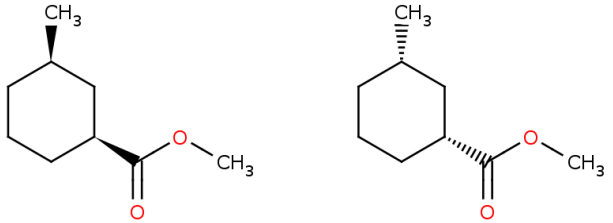
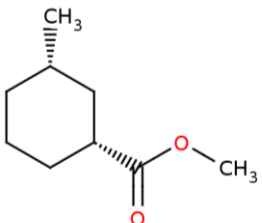
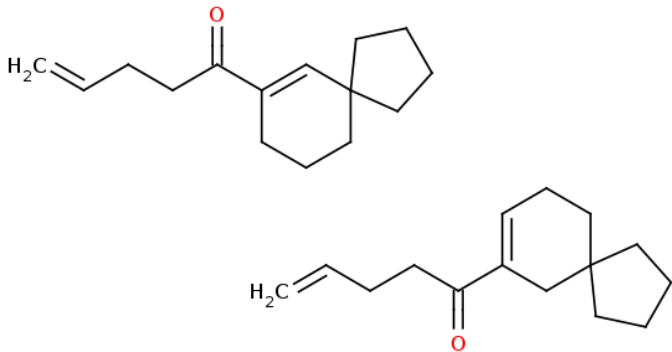
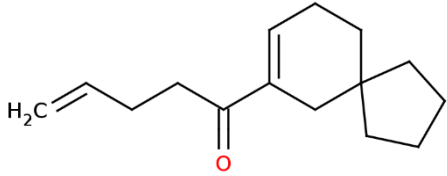
1) Inconsistency related to the molecular structure itself

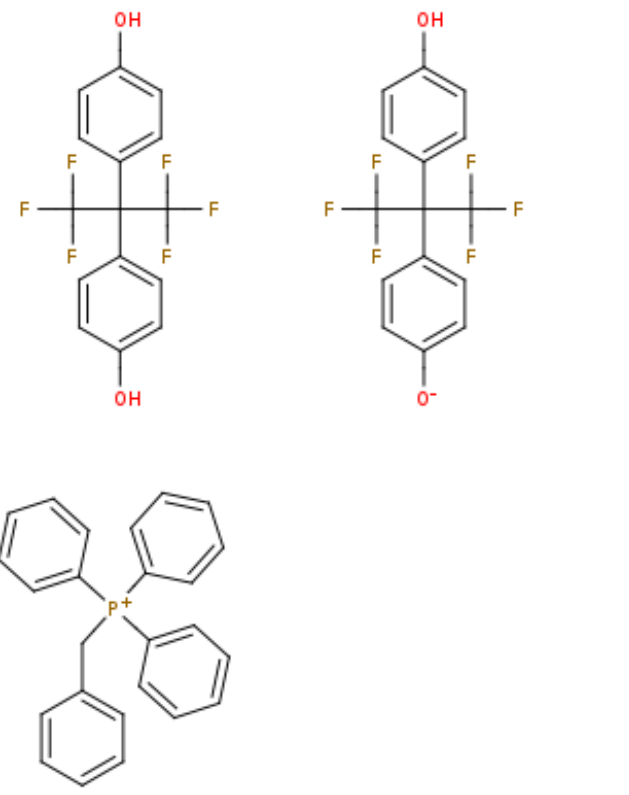
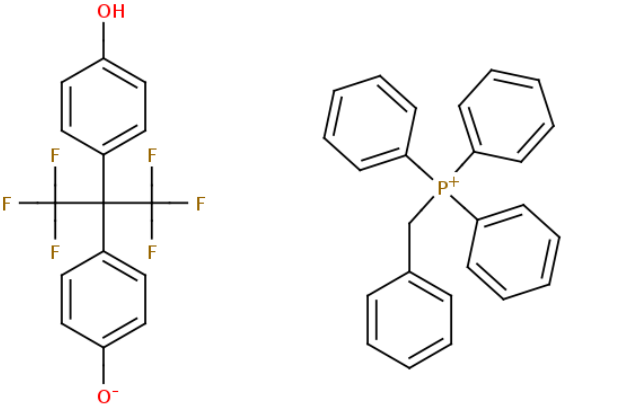
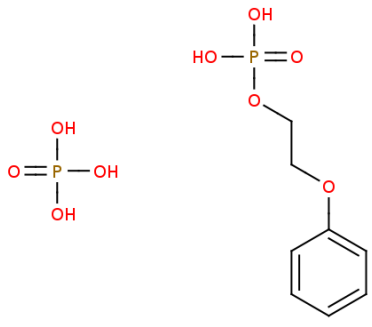
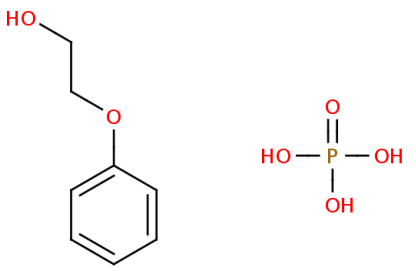
Table 1: Substances in the ECHA database where the SMILES do not correspond to the Chemical Abstract Service Registry Number™ (CAS RN™) as allocated in SciFinderⁿ. The reason for the mismatch is here the structures itself.

CAS RN™	Structure in the database	Structure corresponding to the CAS RN™	Comment
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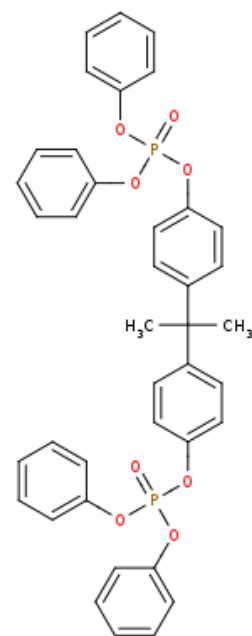
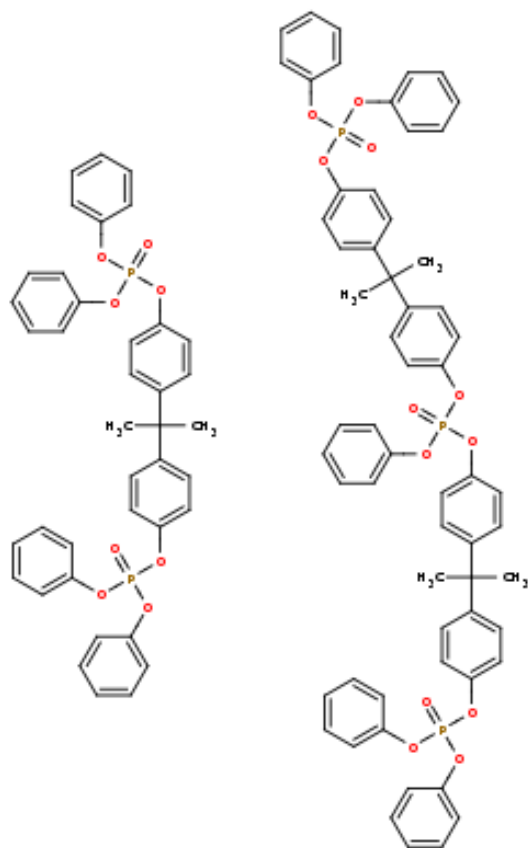
910463-51-3			EC number 459-980-7
1064082-81-0			EC number 805-722-7
17339-74-1	 		EC number 466-270-0 “correct” structure has still missing stereoinforma tion

120218-34-0			EC number 404-440-8
1001252-30-7			EC number 482-030-8
647828-16-8			EC number 449-360-4

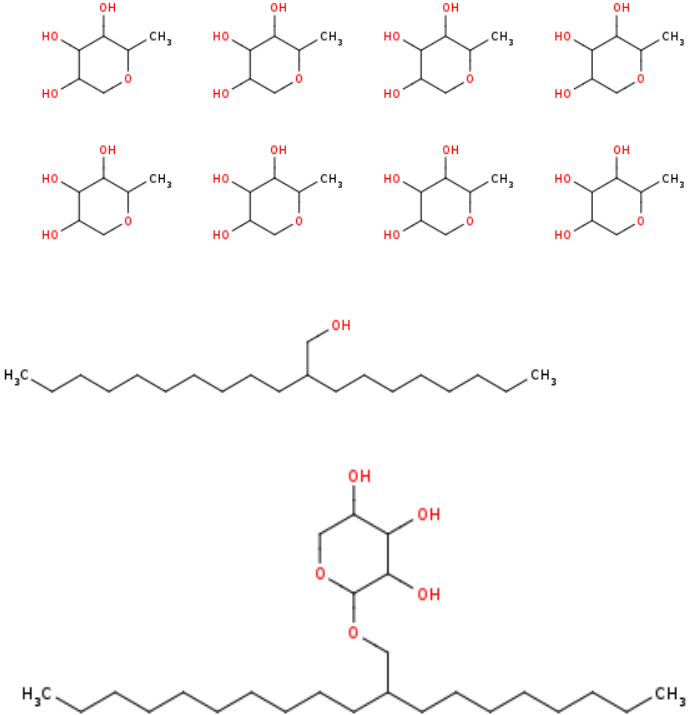
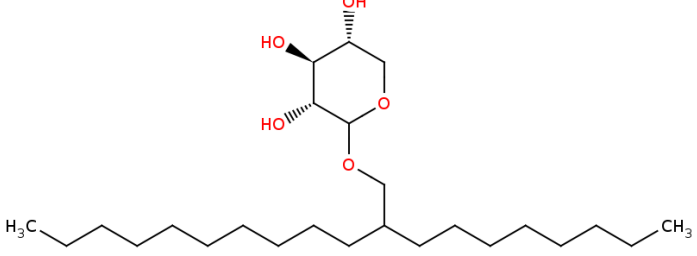
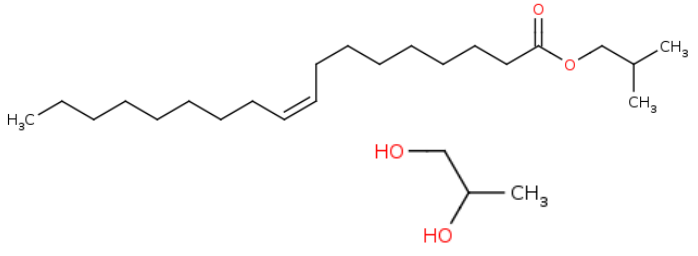
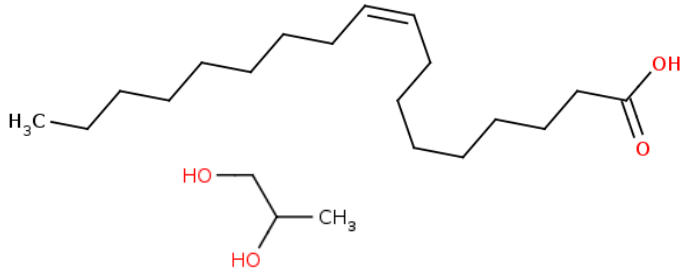
7605-52-9			EC number 700-420-0
224031-70-3			EC number 438-060-9

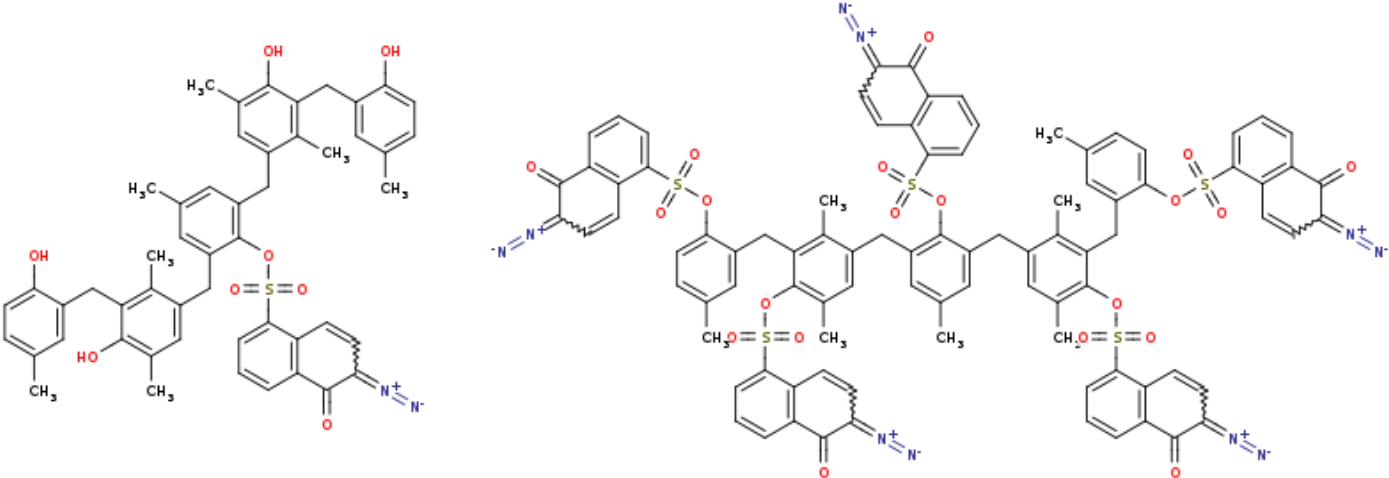
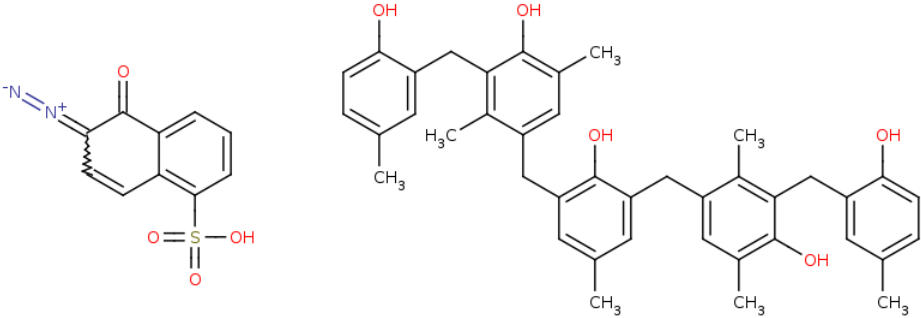
75768-65-9	 Chemical structures of 2,2-bis(4-hydroxyphenyl)hexafluoropropane and 2,2-bis(4-hydroxyphenyl)hexafluoroethane, and triphenylmethyl phosphonium salt.	 Chemical structures of 2,2-bis(4-hydroxyphenyl)hexafluoroethane and triphenylmethyl phosphonium salt.	EC number 278-305-5
39464-70-5	 Chemical structures of phosphoric acid and 2-((benzyloxy)phosphoryl)ethanol.	 Chemical structures of benzyl alcohol and phosphoric acid.	EC number 609-691-9

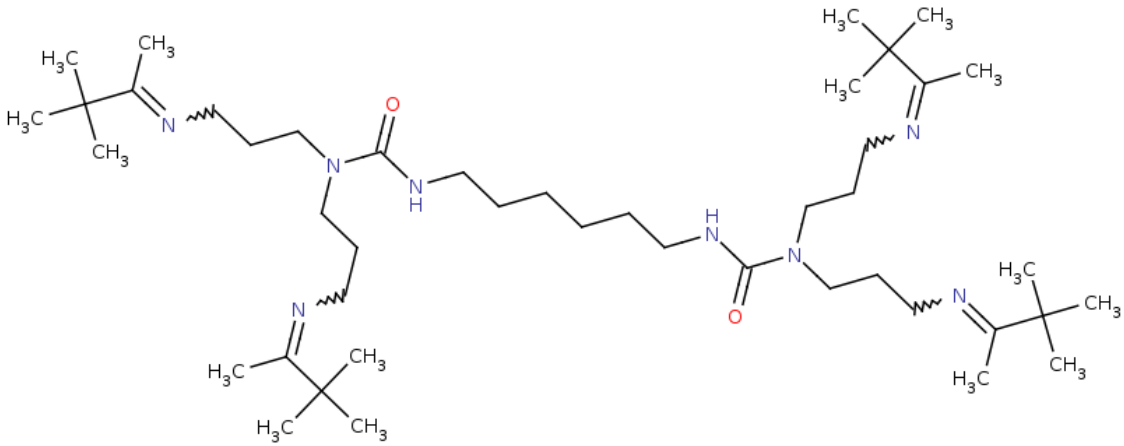
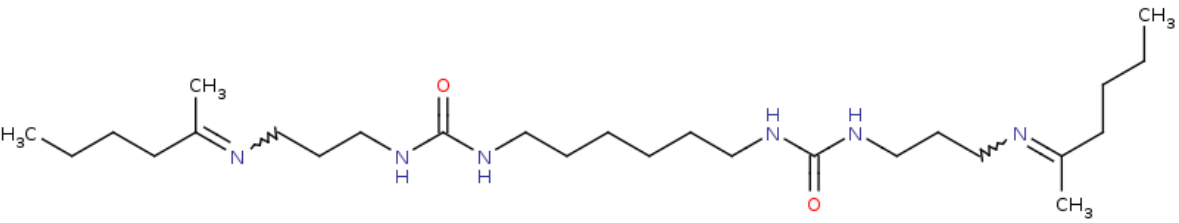
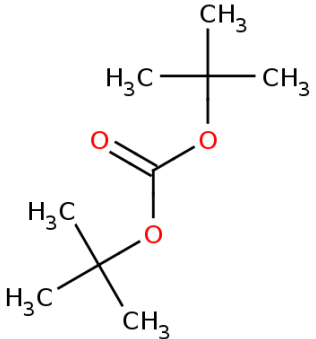
5945-33-5

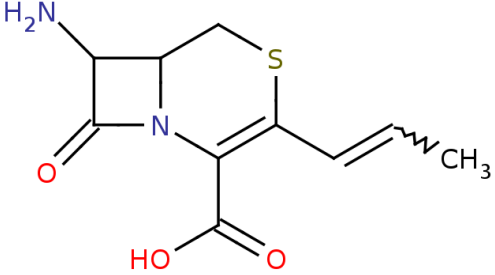
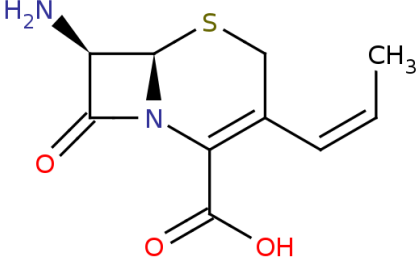
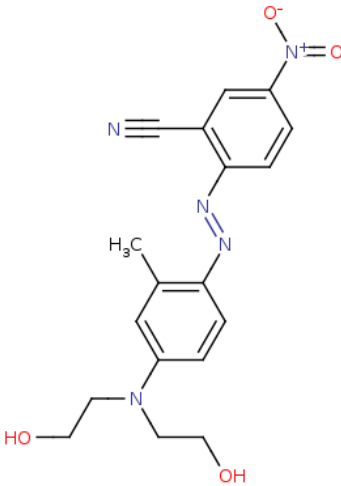
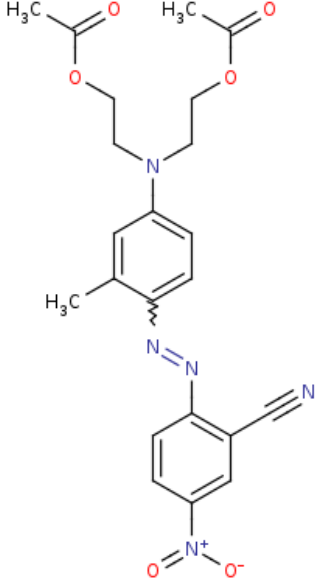


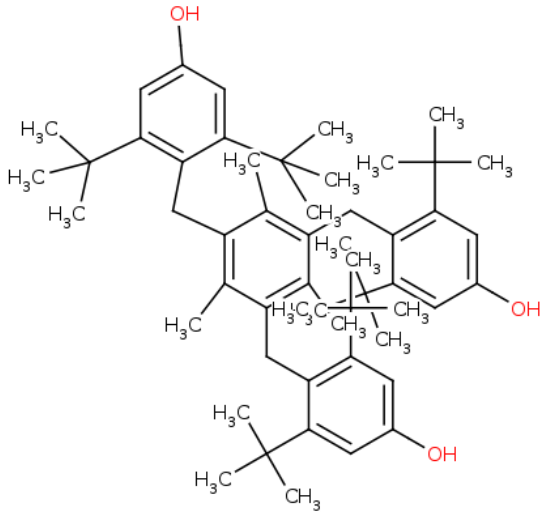
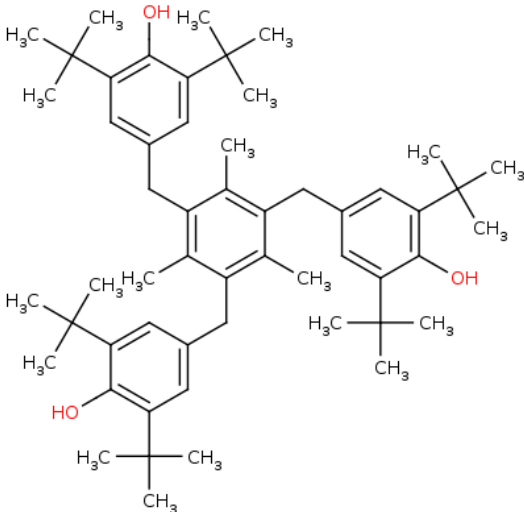
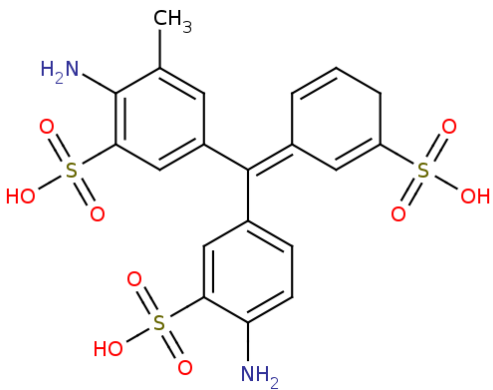
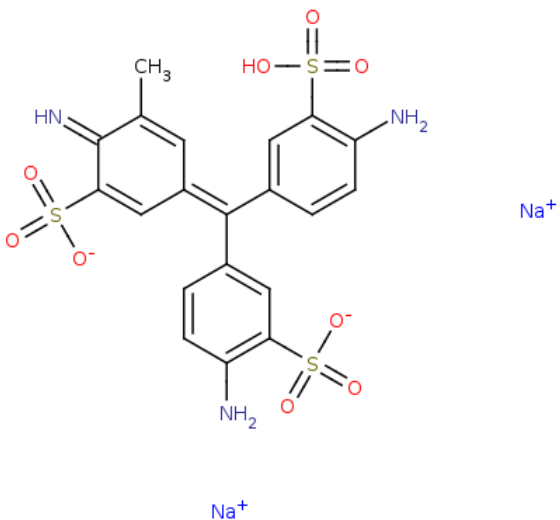
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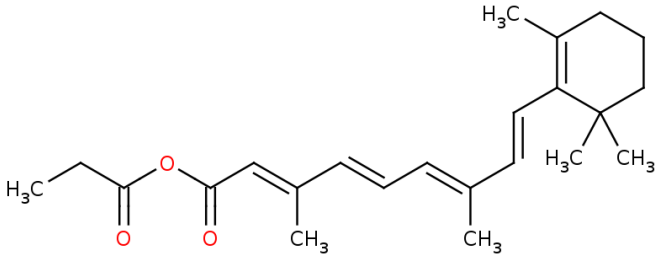
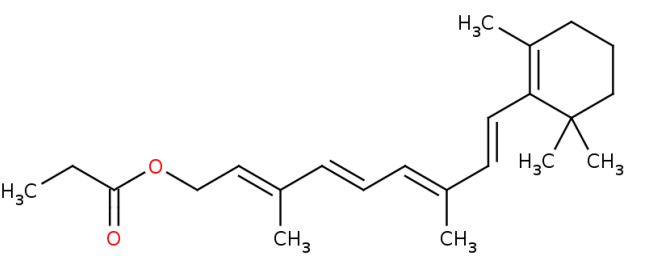
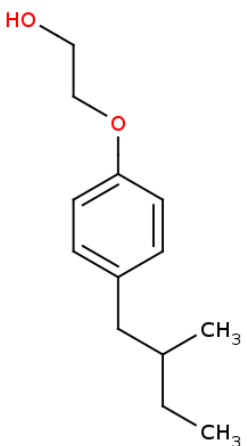
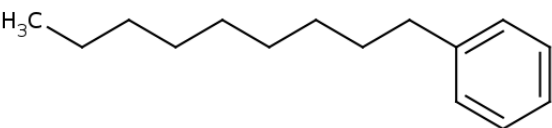
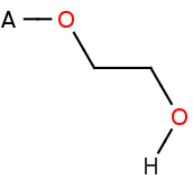
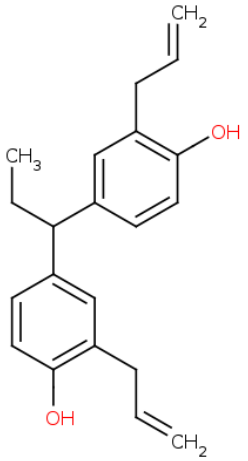
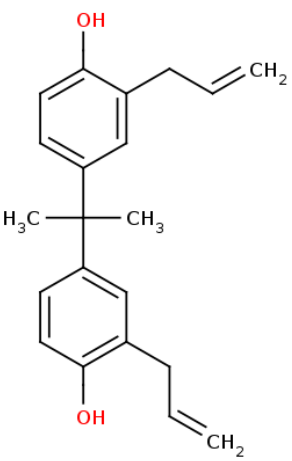
423772-95-6	 Chemical structures for 423772-95-6 include eight pyranose units (each with red OH and CH₃ groups), a long-chain alcohol (H₃C-(CH₂)₁₆-CH₂-OH), and a long-chain glycoside (H₃C-(CH₂)₁₆-CH₂-O-pyranose).	 Chemical structure for 423772-95-6: A long-chain glycoside (H₃C-(CH₂)₁₆-CH₂-O-pyranose) with a pyranose unit and a long alkyl chain.	EC number 464-320-6
1330-80-9	 Chemical structures for 1330-80-9 include a long-chain alcohol (H₃C-(CH₂)₁₆-CH₂-OH), a long-chain glycoside (H₃C-(CH₂)₁₆-CH₂-O-pyranose), and a long-chain alcohol with a hydroxyl group (H₃C-(CH₂)₁₆-CH₂-OH).	 Chemical structure for 1330-80-9: A long-chain alcohol with a hydroxyl group (H₃C-(CH₂)₁₆-CH₂-OH) and a long-chain glycoside (H₃C-(CH₂)₁₆-CH₂-O-pyranose).	EC number 215-549-3

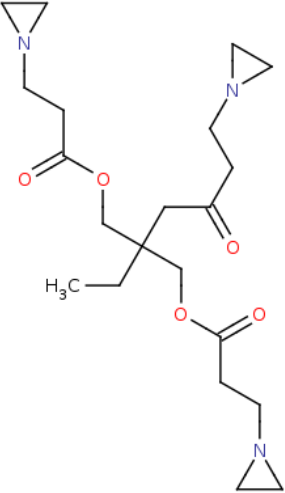
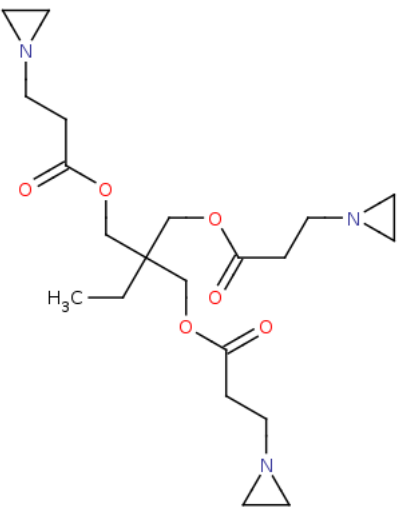
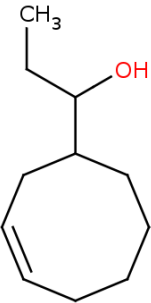
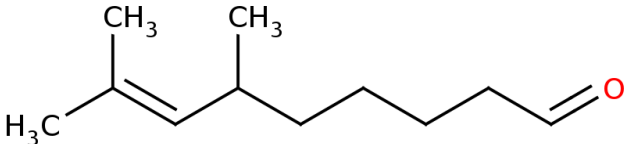
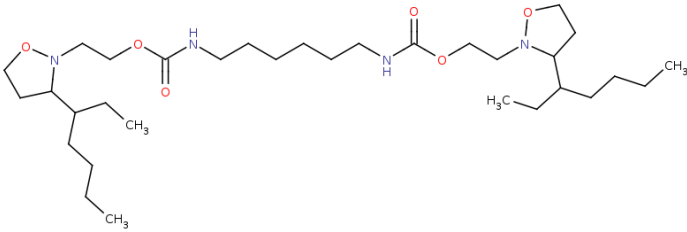
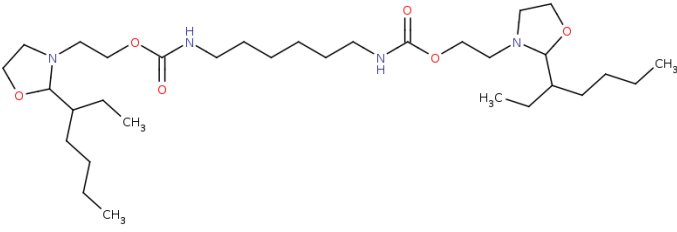
190394-85-5 (incorrect)		EC number 466-400-6
190394-85-5 (correct)		EC number 466-400-6

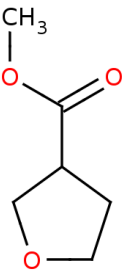
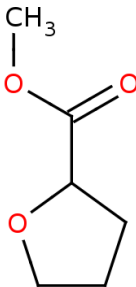
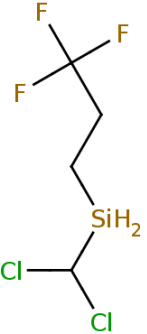
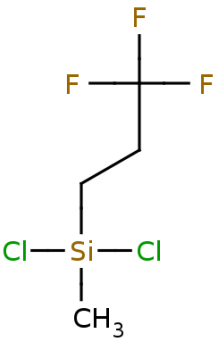
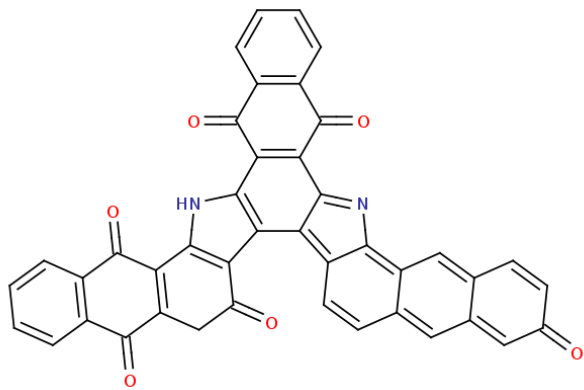
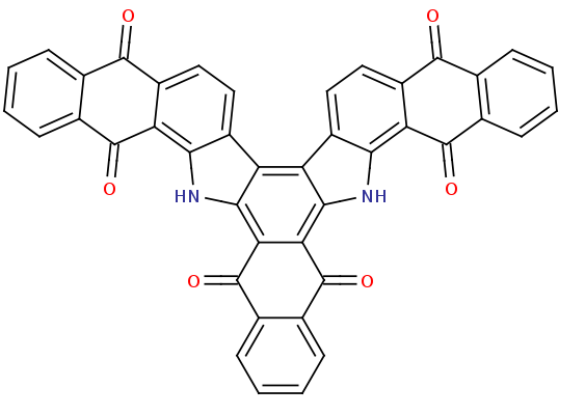
771478-66-1 (incorrect)	 The structure shows a central chain of amide and amine groups. From left to right: a tert-butyl group connected to a methylene group, which is connected to a nitrogen atom. This nitrogen is part of a tertiary amine that also connects to another methylene group and an amide group. The amide group connects to a long methylene chain, which then connects to another amide group. This second amide group connects to a nitrogen atom, which is part of a tertiary amine that also connects to a methylene group and an amide group. Finally, this amide group connects to a tert-butyl group. There are also two other tert-butyl groups connected to the central chain via amine linkers.	EC number 420-190-2
771478-66-1 (correct)	 The structure shows a central chain of amide and amine groups. From left to right: a tert-butyl group connected to a methylene group, which is connected to a nitrogen atom. This nitrogen is part of a tertiary amine that also connects to another methylene group and an amide group. The amide group connects to a long methylene chain, which then connects to another amide group. This second amide group connects to a nitrogen atom, which is part of a tertiary amine that also connects to a methylene group and an amide group. Finally, this amide group connects to a tert-butyl group. There are also two other tert-butyl groups connected to the central chain via amine linkers.	EC number 420-190-2
24424-99-5	 The structure shows two tert-butyl groups connected by an ester linkage. The left tert-butyl group is connected to an oxygen atom, which is part of an ester group. The right tert-butyl group is also connected to an oxygen atom, which is part of an ester group. The two ester groups are connected by a central carbon atom.	EC number 246-240-1

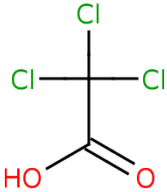
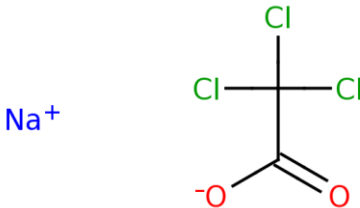
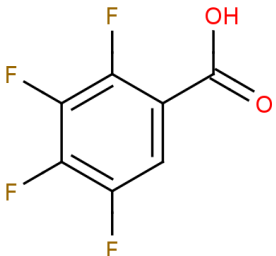
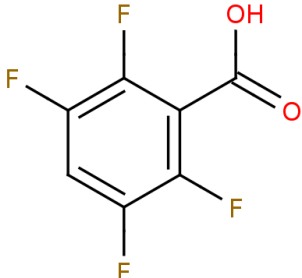
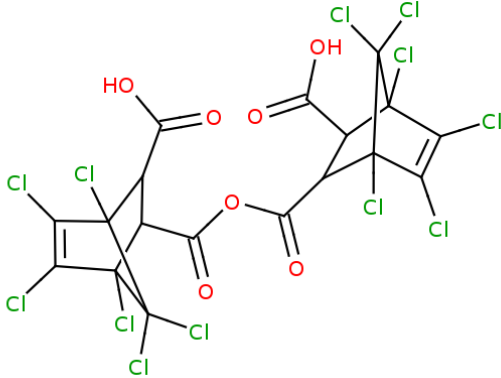
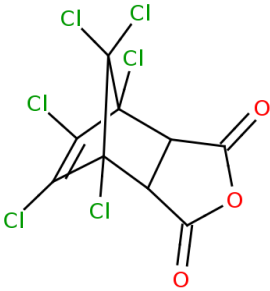
106447-44-3			EC number 415-750-8
12236-25-8			EC number 235-460-3

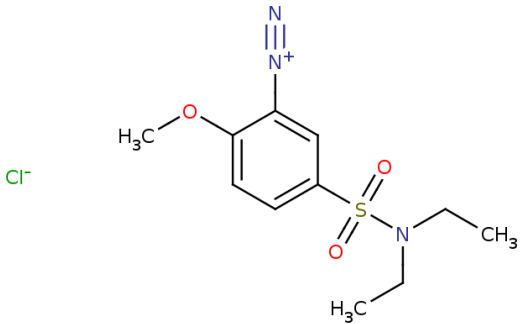
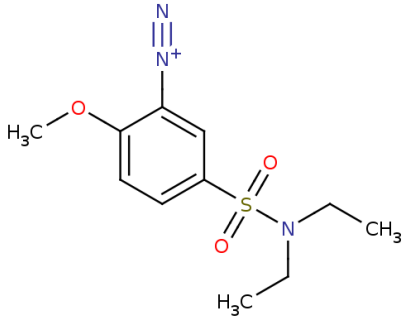
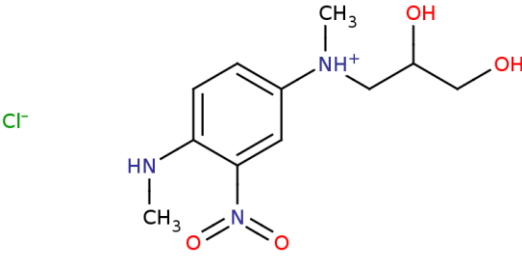
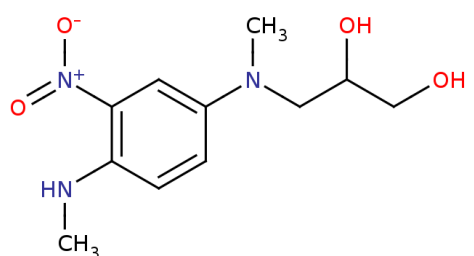
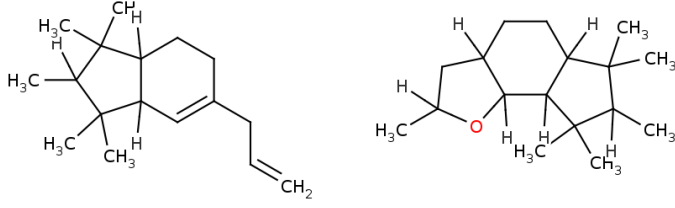
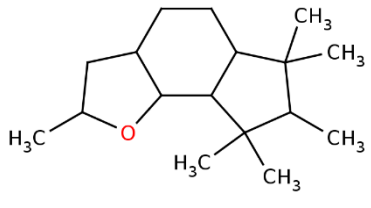
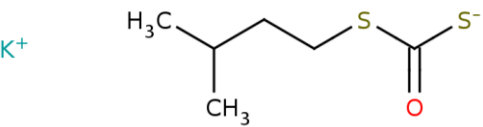
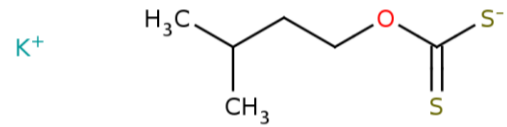
1709-70-2	 Chemical structure of a complex polycyclic compound, likely a steroid derivative, featuring multiple methyl groups (CH₃) and hydroxyl groups (OH) in red.	 Chemical structure of a complex polycyclic compound, likely a steroid derivative, featuring multiple methyl groups (CH₃) and hydroxyl groups (OH) in red.	EC number 216-971-0
3244-88-0	 Chemical structure of a complex molecule featuring multiple sulfonamide groups (SO₂NH₂) and an amine group (NH₂) in blue.	 Chemical structure of a complex molecule featuring multiple sulfonamide groups (SO₂NH₂) and an amine group (NH₂) in blue. The structure includes sodium ions (Na⁺) in blue.	EC number 221-816-5

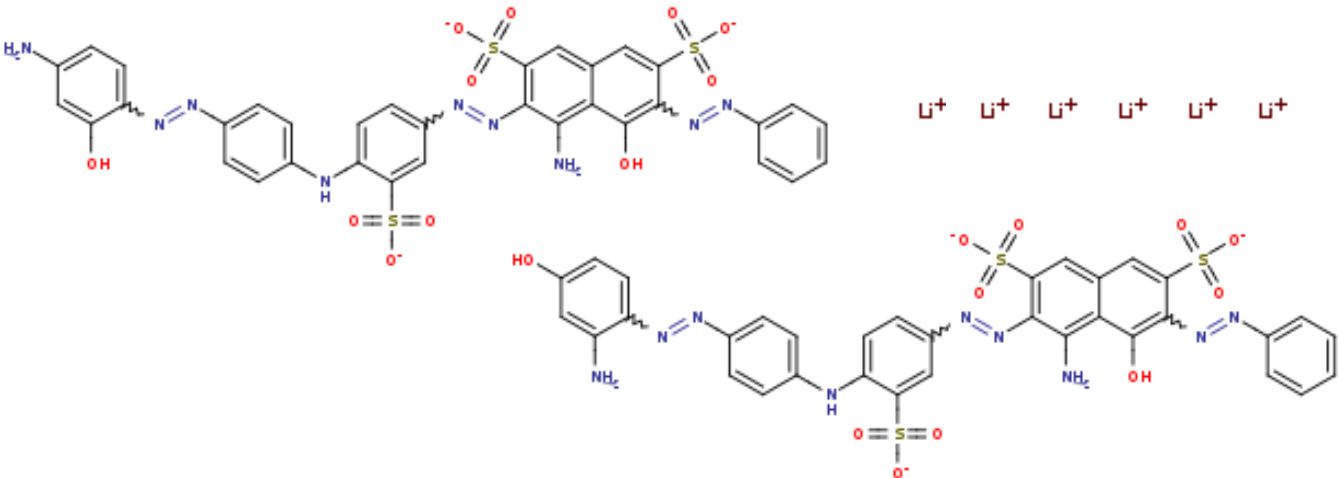
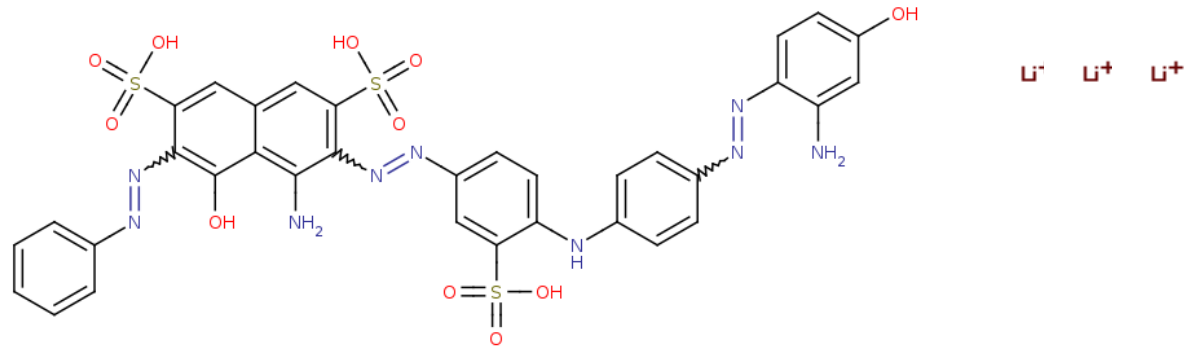
7069-42-3	 Chemical structure of a long-chain unsaturated ester. The chain consists of a methyl group, an ester group, a methylene group, and a series of conjugated double bonds. The chain ends with a cyclohexene ring substituted with two methyl groups.	 Chemical structure of a long-chain unsaturated ester, identical to the one in the previous cell.	EC number 230-363-2
9016-45-9	 Chemical structure of 4-(2-ethylphenyl)butan-1-ol. It features a benzene ring with an ethyl group at the 2-position and a 4-hydroxybutyl group at the 1-position.	CAS RN represents polymer with the monomer units shown here   Second molecule is somewhere attached to the first one. The attachment point is 'A'	EC number 500-024-6
1745-89-7	 Chemical structure of 1-(4-hydroxy-3-(prop-1-en-1-yl)phenyl)propan-2-ol. It features a benzene ring with a hydroxyl group at the 4-position and a prop-1-en-1-yl group at the 3-position. The ring is attached to a 1-hydroxypropan-2-yl group.	 Chemical structure of 1-(4-hydroxy-3-(prop-1-en-1-yl)phenyl)propan-2-ol, identical to the one in the previous cell.	EC number 217-121-1

52234-82-9			EC number 257-765-0
899810-84-5			EC number 476-140-5
140921-24-0			EC number 411-700-4

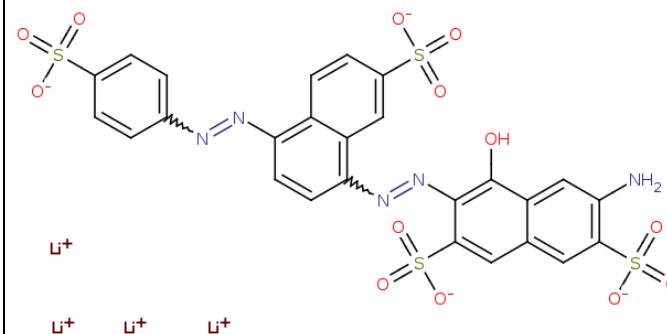
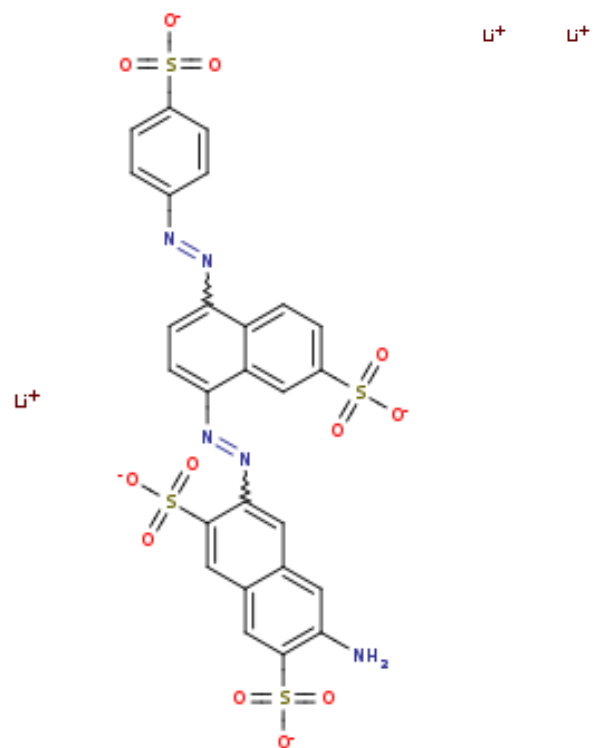
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2475-33-4			EC number 219-599-7

650-51-1			EC number 211-479-2
652-18-6			EC number 435-890-3
115-27-5			EC number 204-077-3

27580-14-9			EC number 248-543-4
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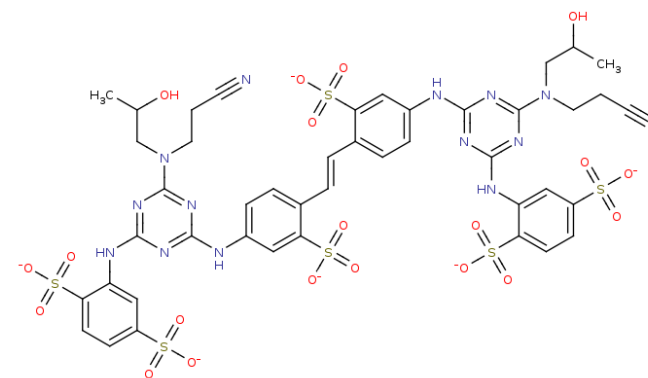
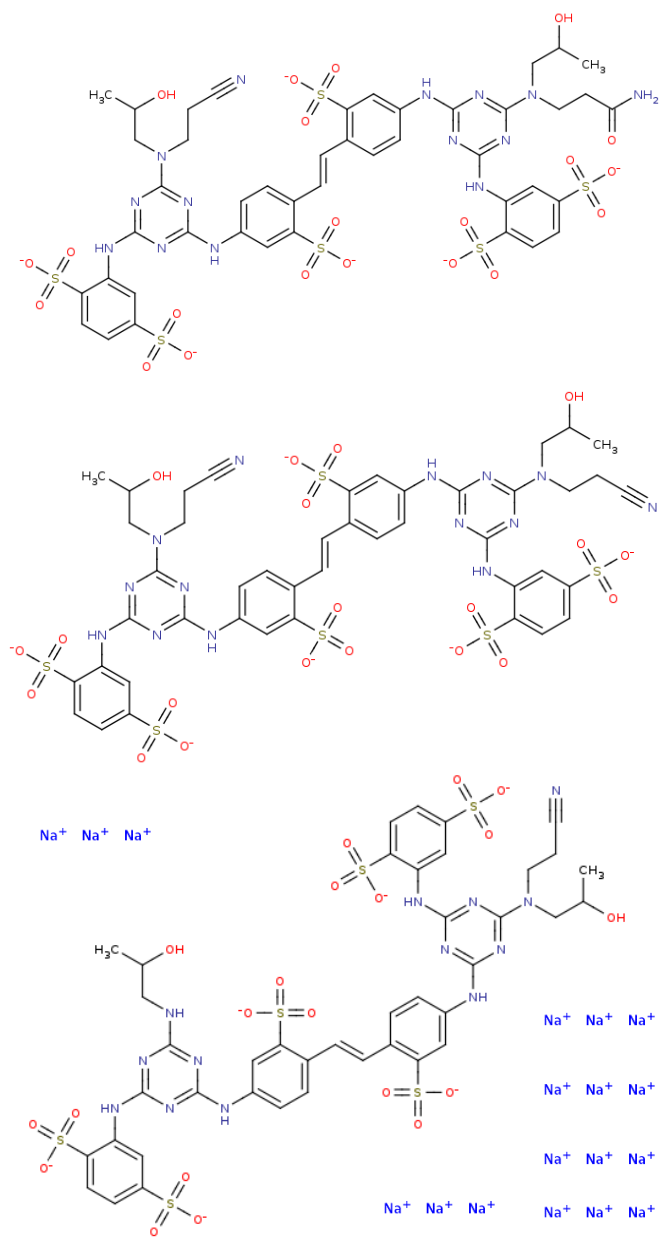
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106028-58-4



EC number
405-150-4

76508-02-6

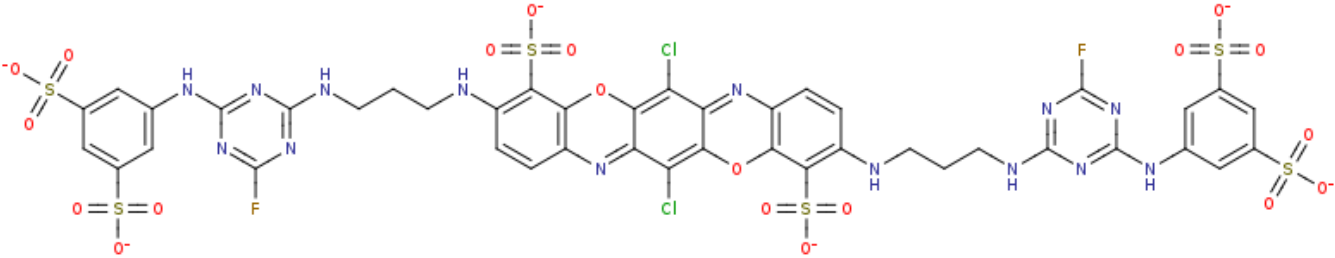
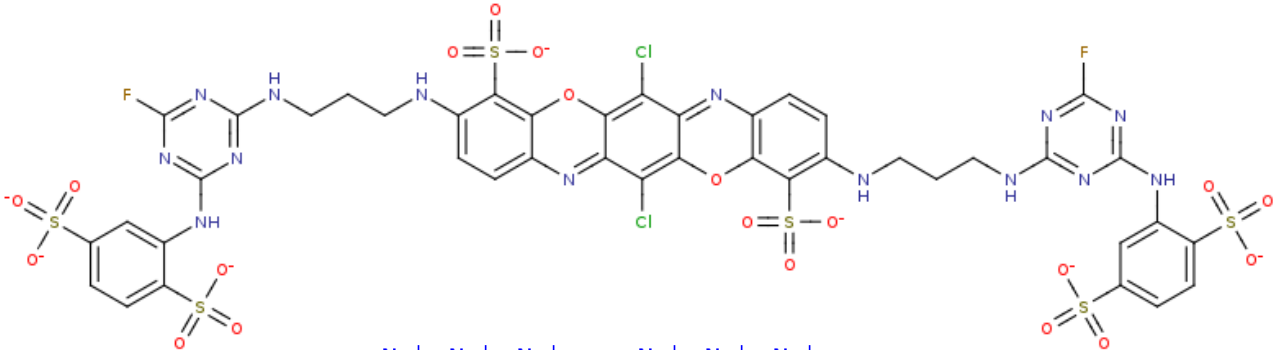


Na⁺ Na⁺ Na⁺

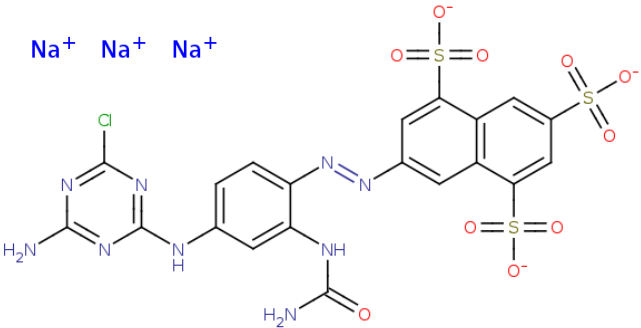
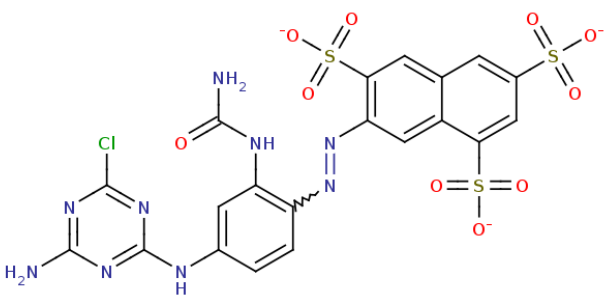
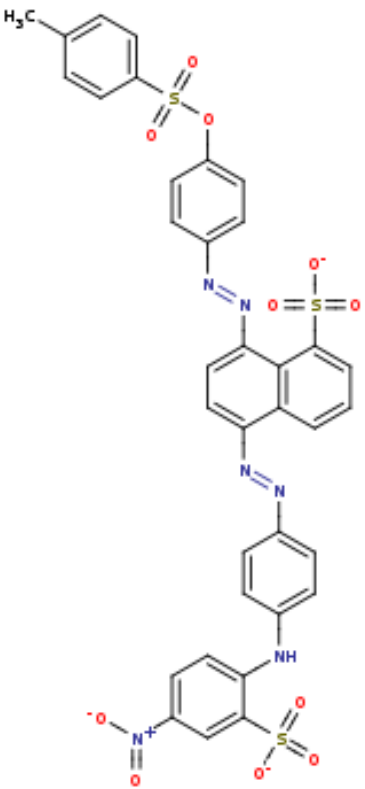
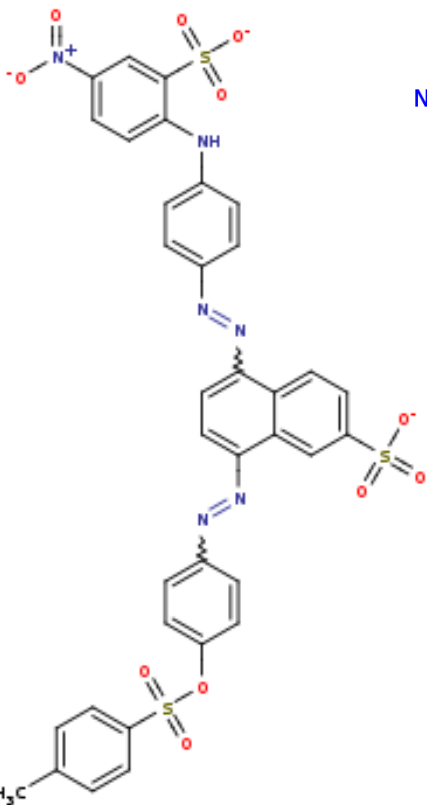
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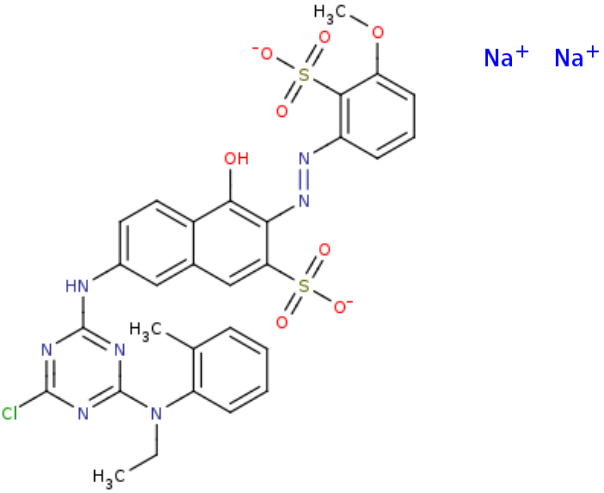
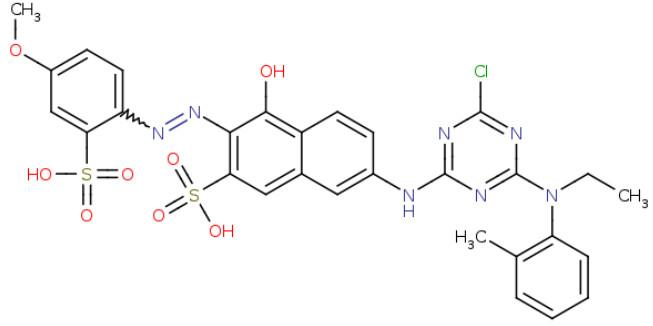
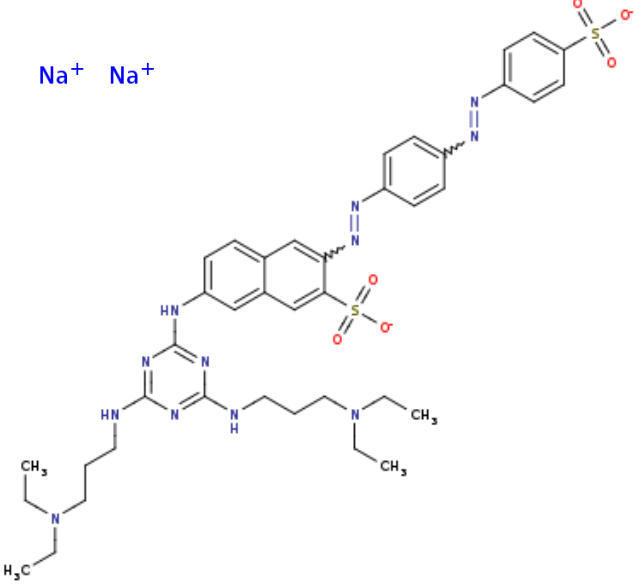
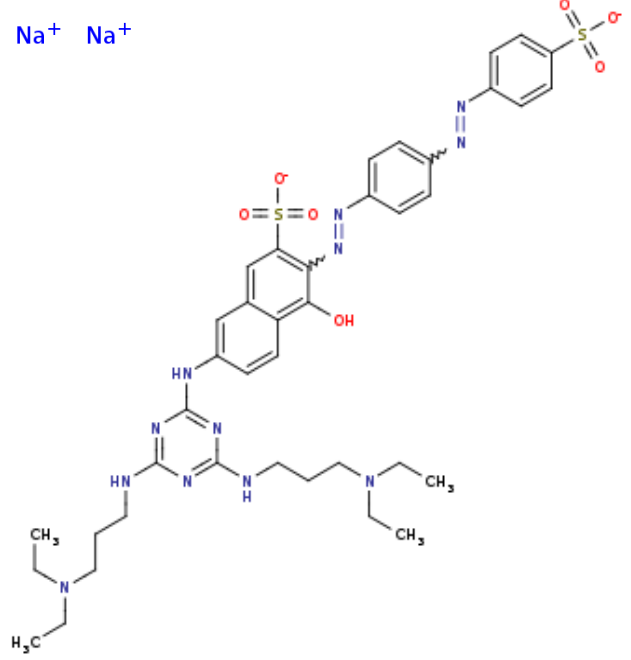
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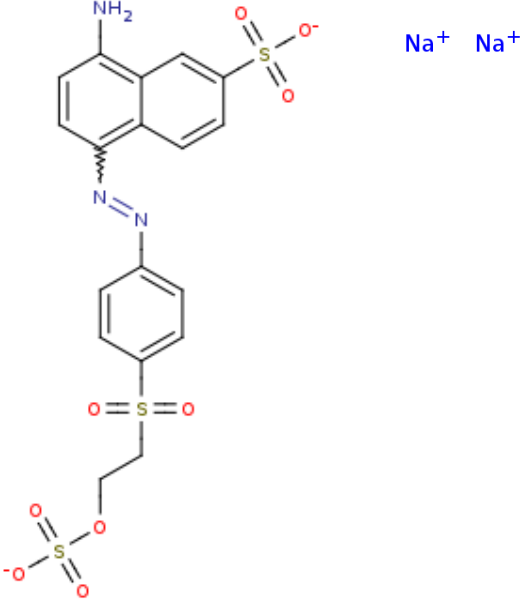
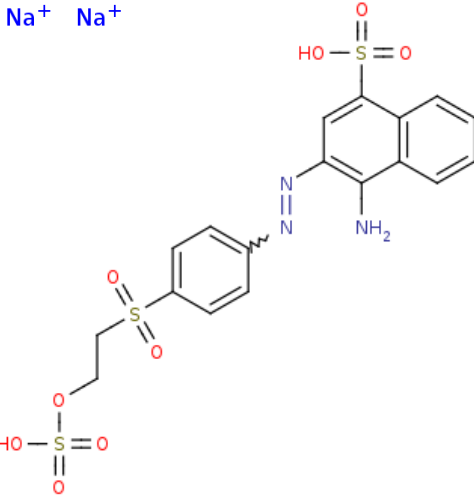
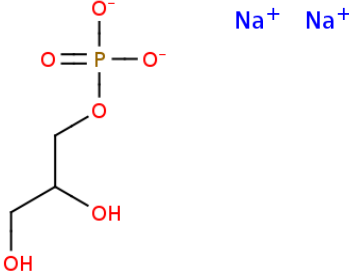
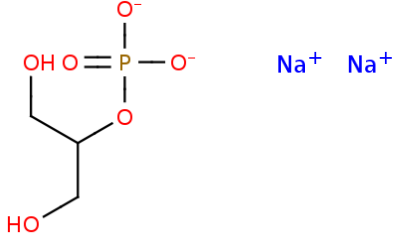
CAS RN™
includes only
the second
structure

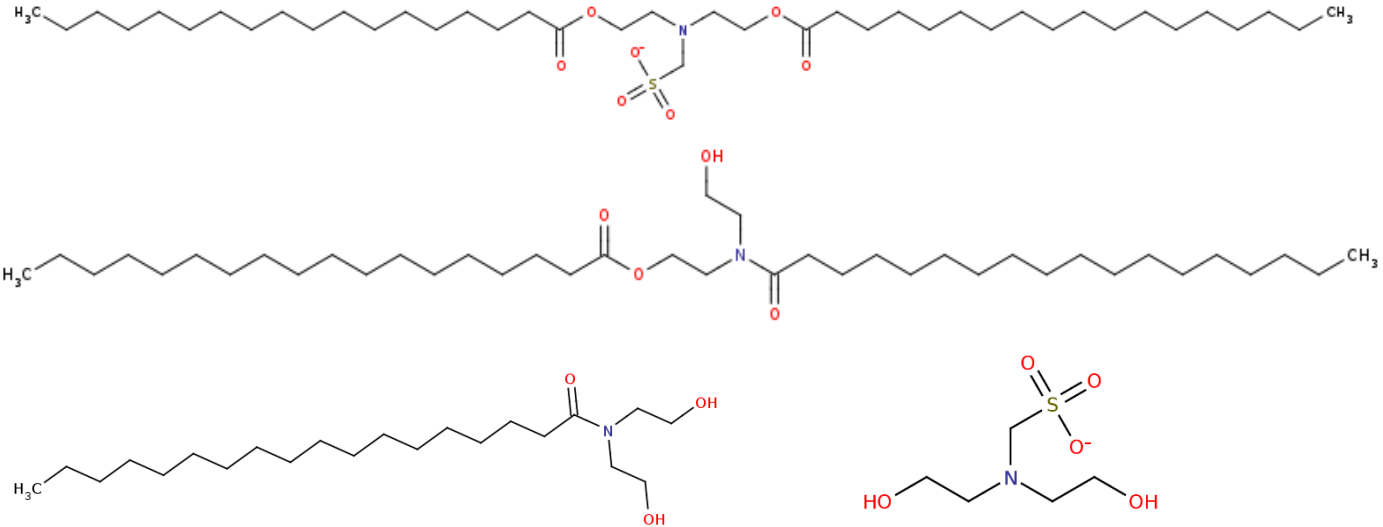
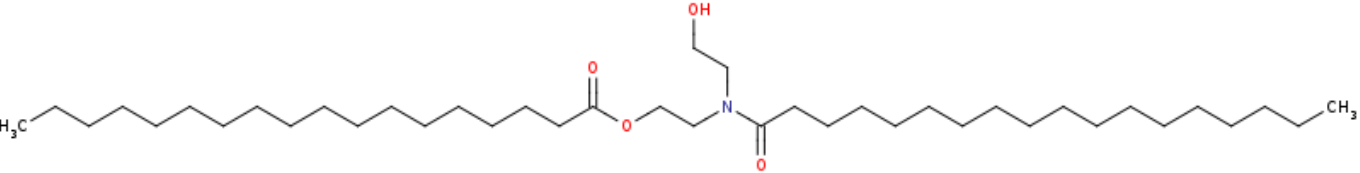
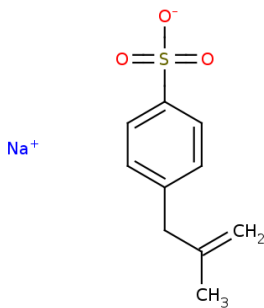
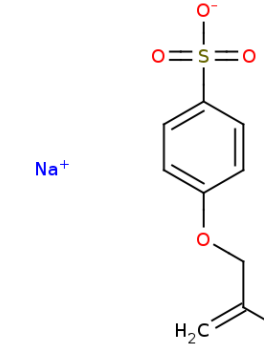
85153-92-0 (incorrect form)	 Na⁺ Na⁺ Na⁺ Na⁺ Na⁺ Na⁺	EC number 400-050-7
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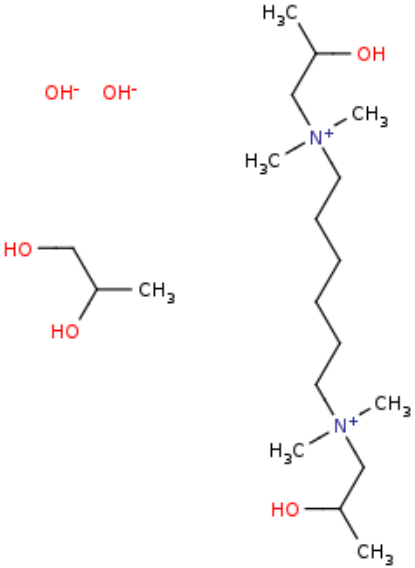
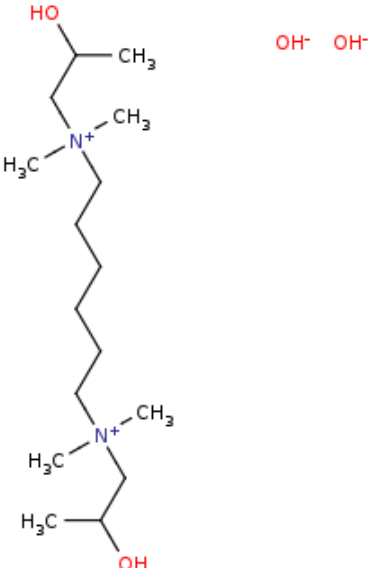
371921-41-4 (incorrect form)	The structure shows a complex molecule with two triazine rings connected by a biphenyl group. Each triazine ring has a 4-sulfamoylphenyl substituent. The biphenyl group is linked to a 4-sulfamoylphenyl ring via a diazo bridge. This ring is further connected to a 4-sulfamoylphenyl ring via a trans-vinyl bridge. The final 4-sulfamoylphenyl ring is connected to a 4-sulfamoylphenyl ring via a diazo bridge. The molecule is shown with four sodium ions (Na+) and four hydroxyl groups (OH) in red. The sulfamoyl groups are shown as SO₂O⁻.	EC number 429-230-3 'correct' form has still missing stereoinforma tion
371921-41-4 (correct form)	The structure shows a complex molecule with two triazine rings connected by a biphenyl group. Each triazine ring has a 4-sulfamoylphenyl substituent. The biphenyl group is linked to a 4-sulfamoylphenyl ring via a diazo bridge. This ring is further connected to a 4-sulfamoylphenyl ring via a trans-vinyl bridge. The final 4-sulfamoylphenyl ring is connected to a 4-sulfamoylphenyl ring via a diazo bridge. The molecule is shown with four sodium ions (Na+) and four hydroxyl groups (OH) in red. The sulfamoyl groups are shown as SO₂OH.	EC number 429-230-3 'correct' form has still missing stereoinforma tion

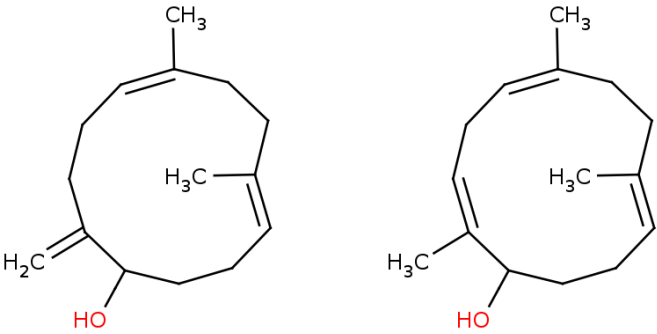
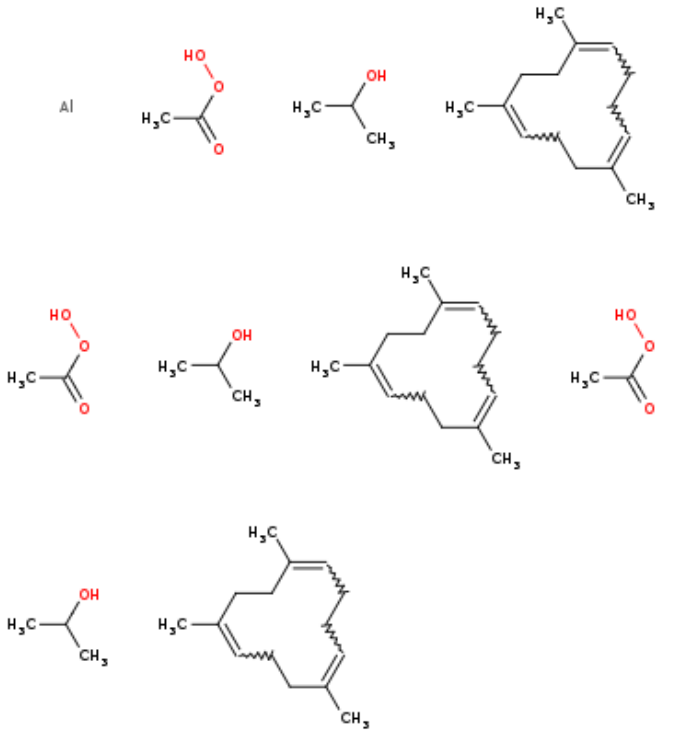
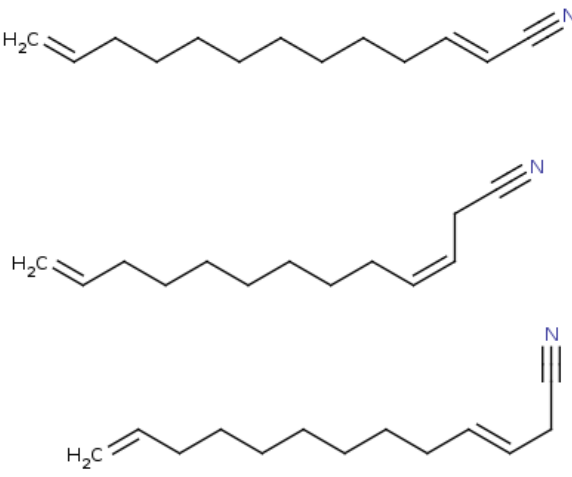
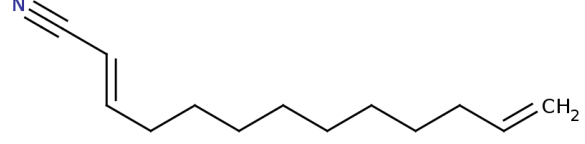
70161-14-7	$\text{Na}^+ \text{Na}^+ \text{Na}^+$ 	 $\text{Na}^+ \text{Na}^+ \text{Na}^+$	EC number 274-349-4
72968-81-1	$\text{Na}^+ \text{Na}^+$ 	$\text{Na}^+ \text{Na}^+$ 	EC number 277-155-8

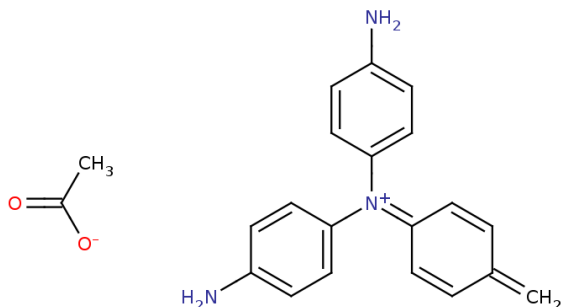
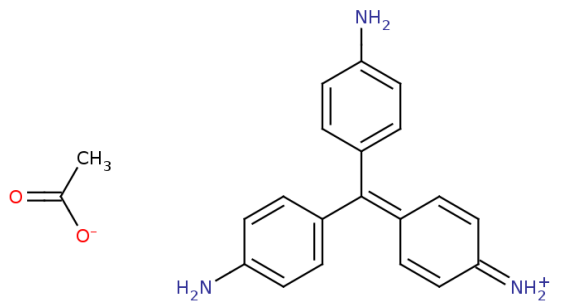
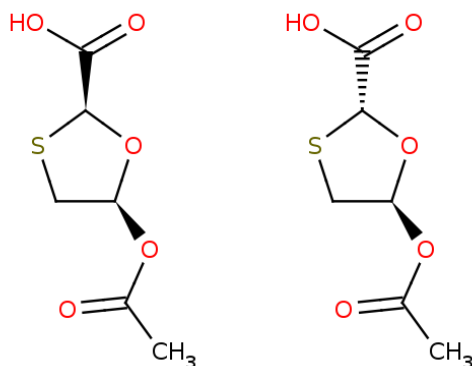
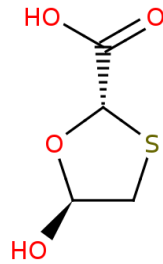
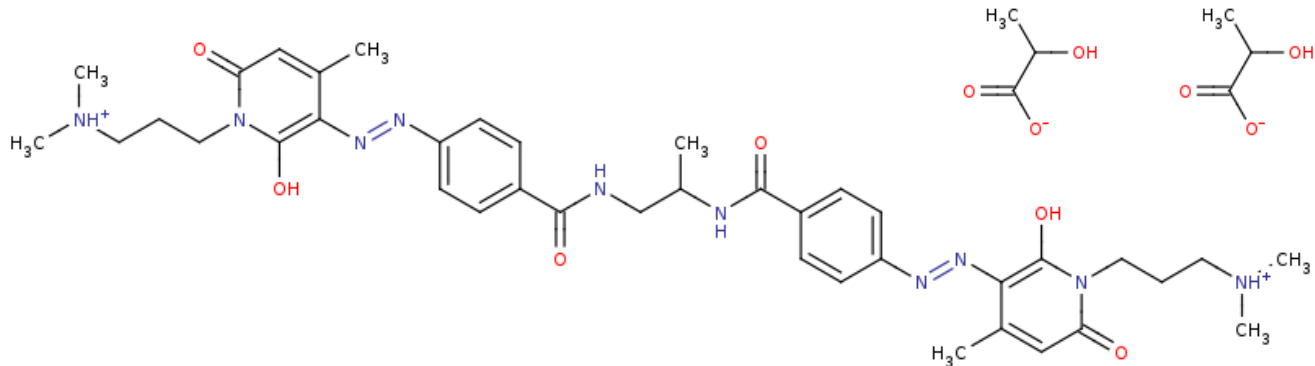
147703-64-8	 Na⁺ Na⁺	 Na⁺ Na⁺	EC number 410-390-8
120029-06-3	 Na⁺ Na⁺	 Na⁺ Na⁺	EC number 419-460-2

250688-43-8			EC number 423-730-5
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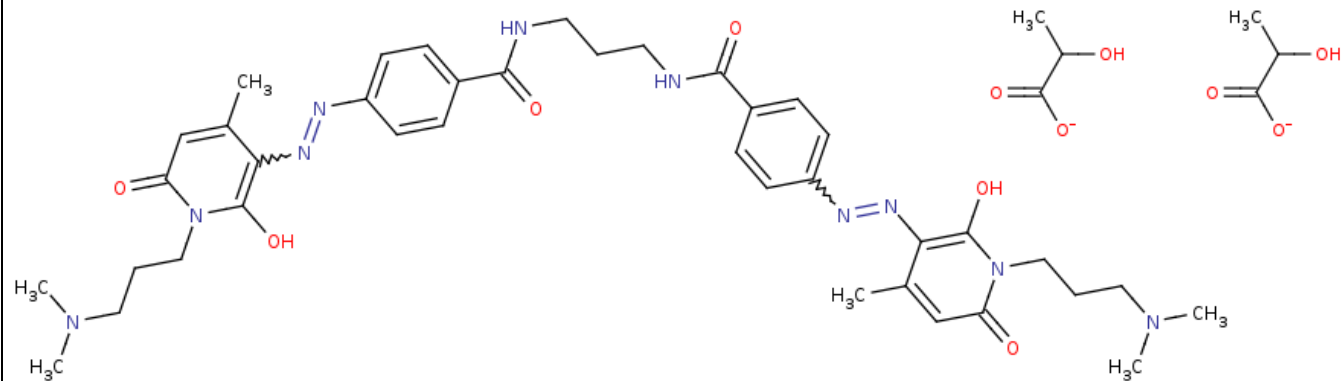
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55349-70-7 (correct form)		EC number 401-230-8 CAS no. contains only second structure
1208-67-9	 	EC number 214-901-3

35132-93-5			EC number 442-730-6 CAS no. does not contain all structural elements
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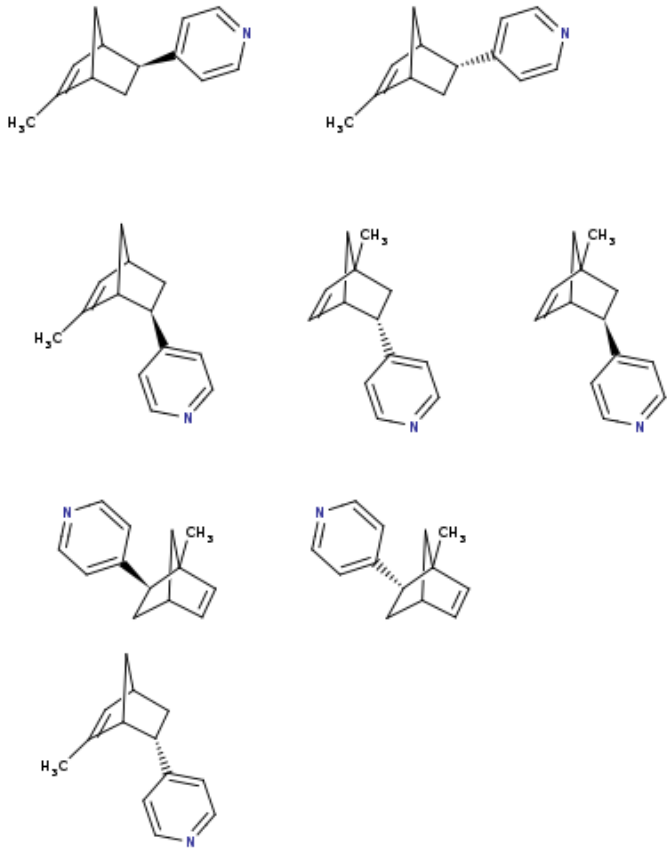
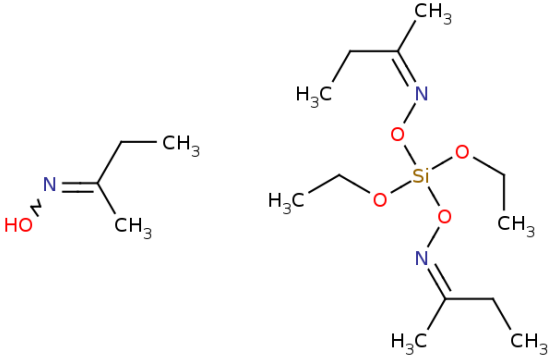
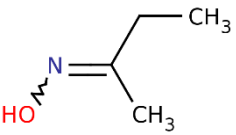
111850-00-1			EC number 413-530-6 'correct' form has still missing stereoinforma tion
124071-40-5			EC number 422-190-8 CAS RN™ contains only the first structure

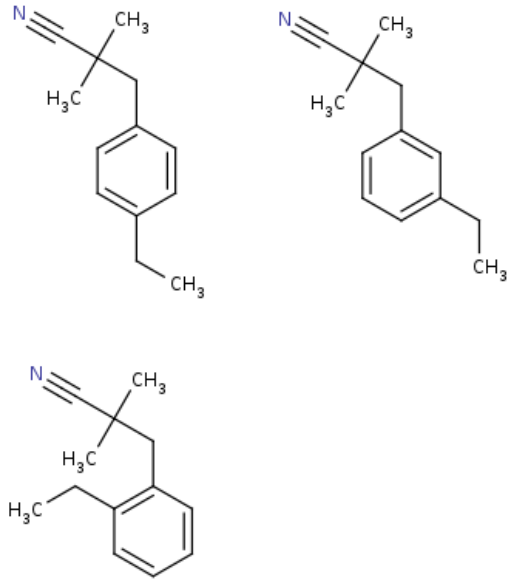
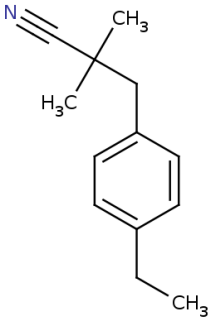
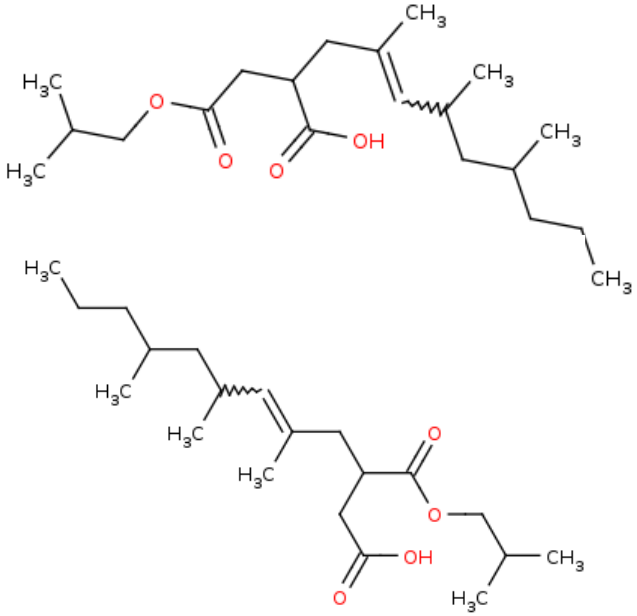
6035-94-5			EC number 227-918-6
147027-04-1			EC number 411-660-8
164578-09-0 (incorrect form)			EC number 403-340-1

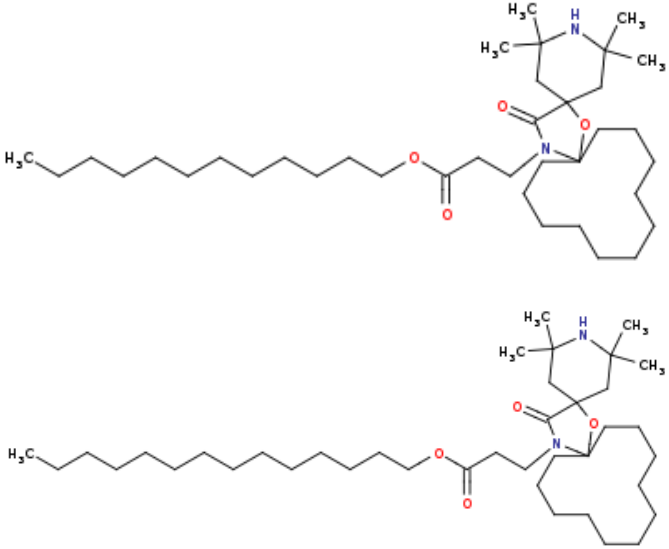
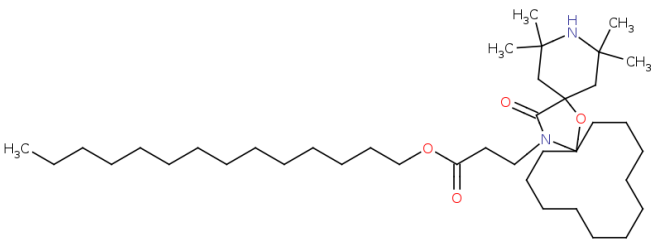
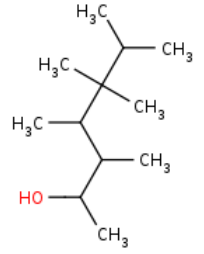
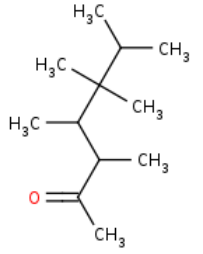
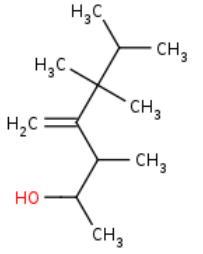
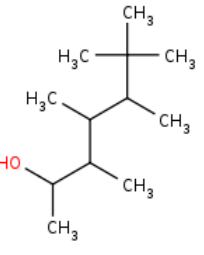
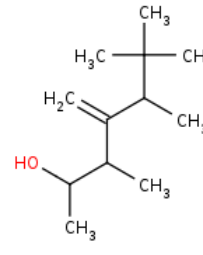
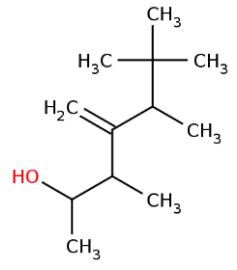
164578-09-0 (correct form)

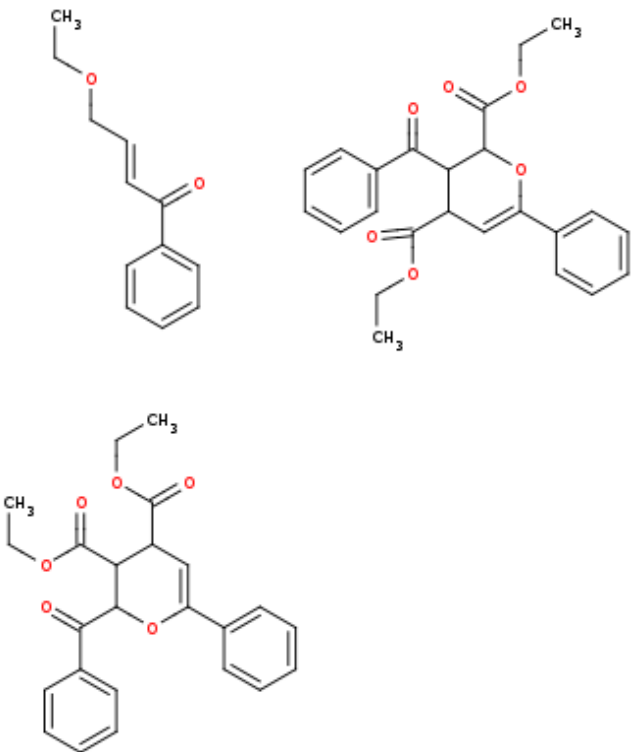
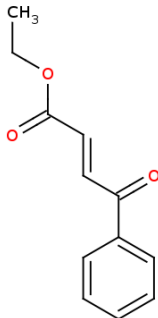
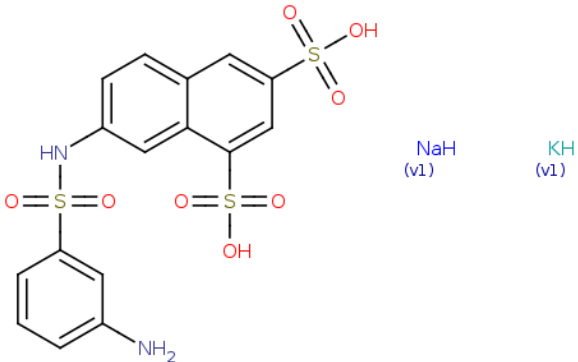


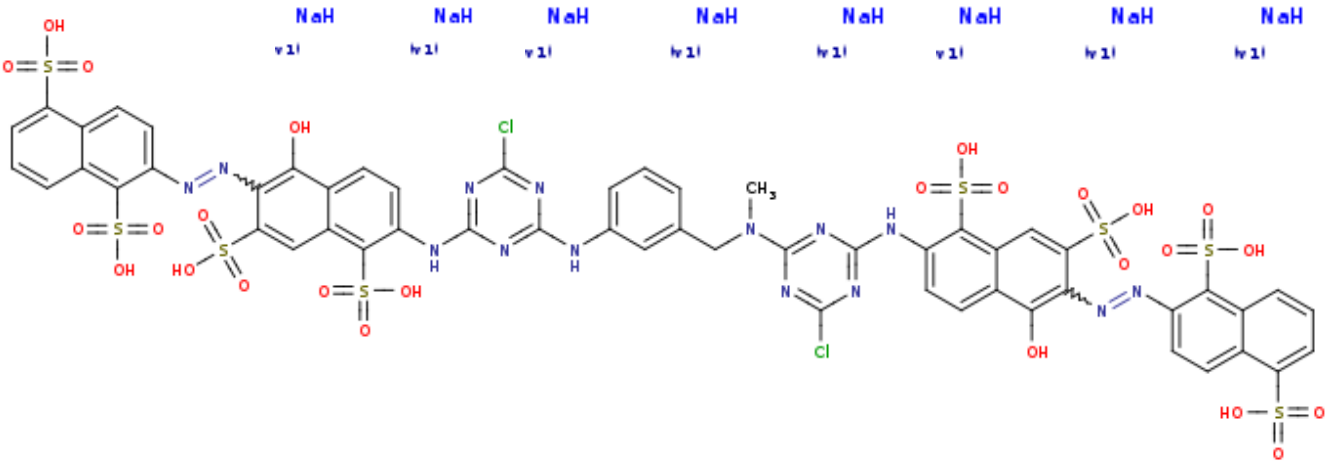
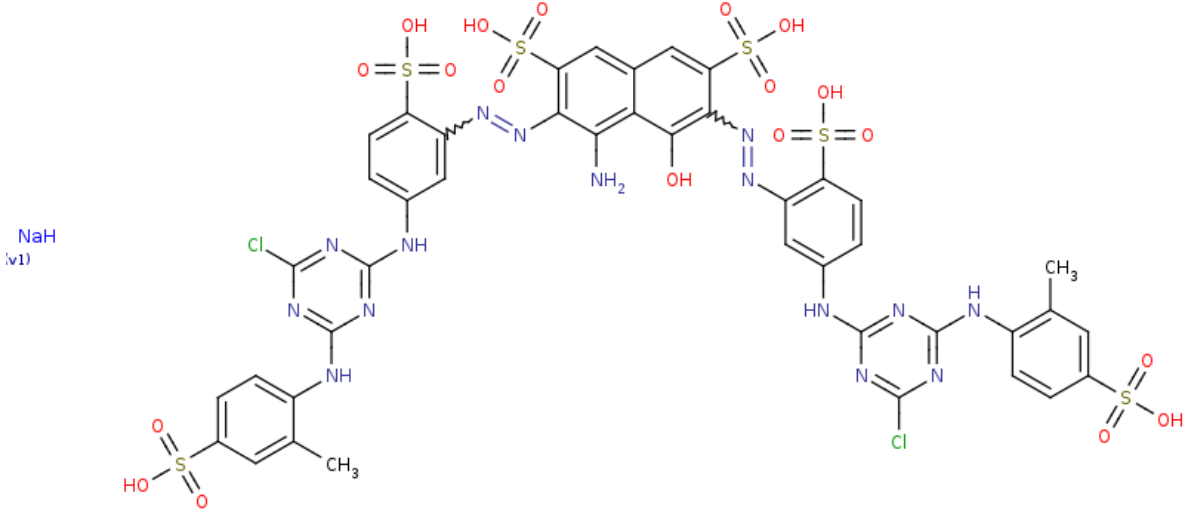
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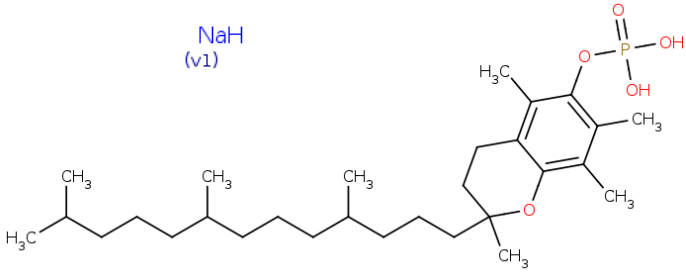
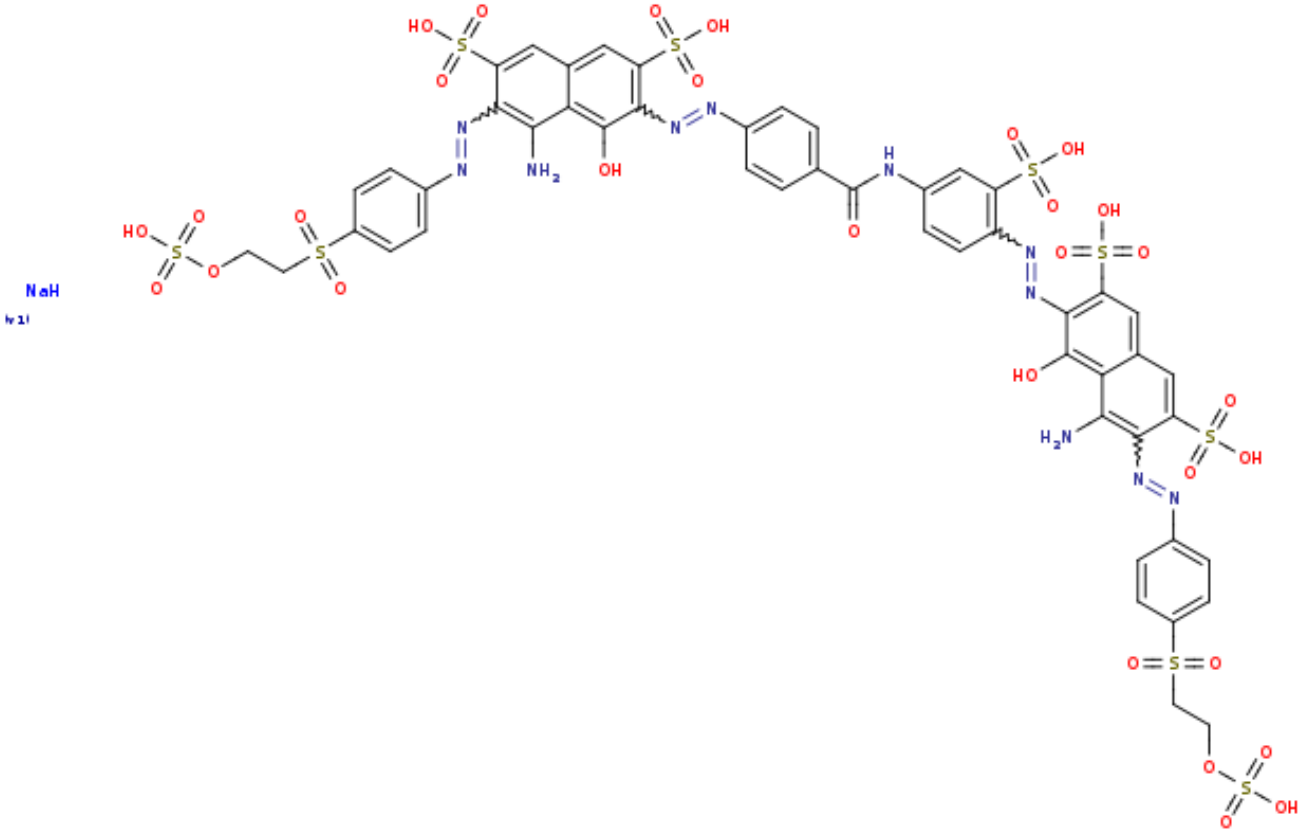
125352-06-9	 Seven chemical structures of bicyclic compounds (bicyclo[2.2.1]hept-2-ene derivatives) substituted with a pyridine ring and a methyl group. The structures show different stereochemical arrangements of the pyridine ring and the methyl group on the bicyclic system.	The components shown in SciFinder do not correspond to the structure elements shown in the ECHA database. However, SciFinder has not the complete structure.	EC number 402-520-7
96-29-7	 Three chemical structures are shown. The first is a hydroxyimino compound (2-methyl-2-butanimine oxime). The second is a siloxane compound (diethyl dimethylsiloxane). The third is a hydroxyimino compound (2-methyl-2-butanimine oxime).	 Chemical structure of a hydroxyimino compound (2-methyl-2-butanimine oxime).	EC number 406-930-7

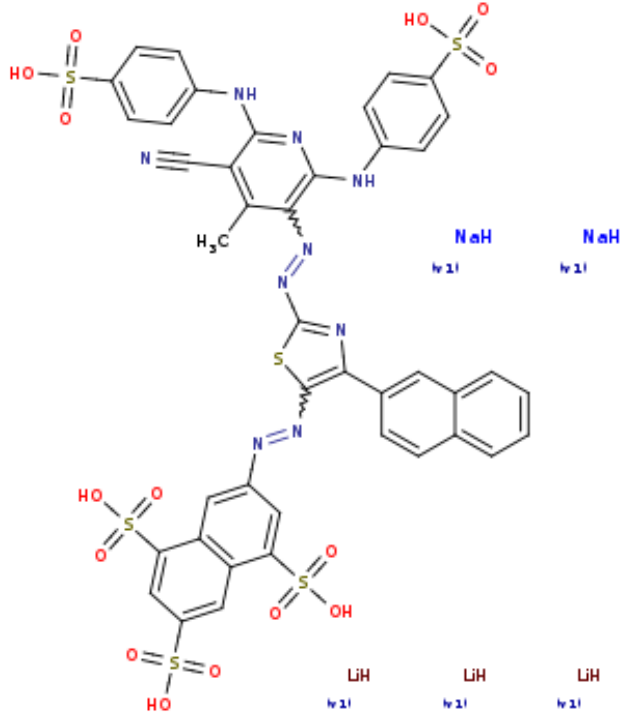
134123-93-6			EC number 412-660-0 CAS RN™ contains only the first structure
141847-13-4		SciFinderⁿ has no final structure but the components do not agree with the ones from the ECHA database	EC number 410-720-0

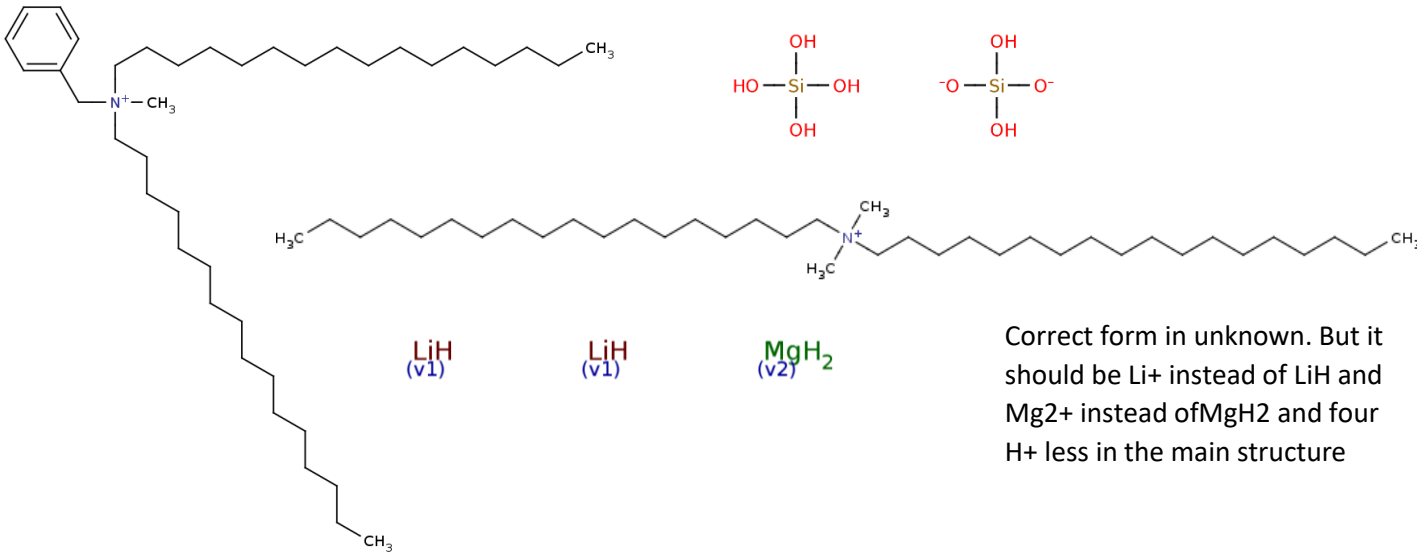
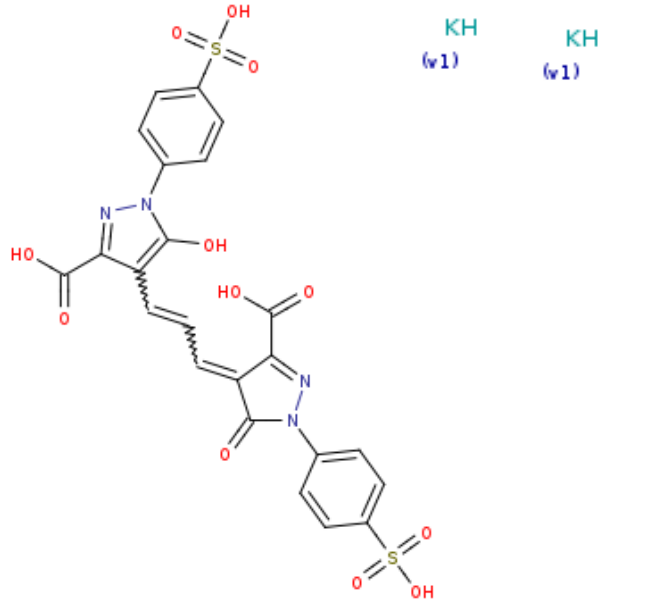
85099-50-9	 The structure shows a long-chain fatty acid (dodecanoic acid) esterified to a complex bicyclic amide system. The bicyclic system consists of a 10-membered ring fused to a 6-membered ring, with a nitrogen atom and a carbonyl group. The nitrogen is substituted with two methyl groups. The carbonyl is part of a five-membered ring. The fatty acid chain is attached to the carbonyl via an ester linkage.	 This structure is identical to the one in the previous cell, showing a long-chain fatty acid ester linked to a complex bicyclic amide system.	EC number 400-580-9 CAS RN™ contains only the second structure
81787-06-6	 Chemical structure of a branched alcohol: 2,3,4-trimethyl-2-pentanol. The hydroxyl group is highlighted in red.  Chemical structure of a branched alcohol: 2,3,4-trimethyl-2-pentanol. The hydroxyl group is highlighted in red.  Chemical structure of a branched alcohol: 2,3,4-trimethyl-2-pentanol. The hydroxyl group is highlighted in red.  Chemical structure of a branched alcohol: 2,3,4-trimethyl-2-pentanol. The hydroxyl group is highlighted in red.  Chemical structure of a branched alcohol: 2,3,4-trimethyl-2-pentanol. The hydroxyl group is highlighted in red.	 Chemical structure of a branched alcohol: 2,3,4-trimethyl-2-pentanol. The hydroxyl group is highlighted in red.	EC number 401-030-0

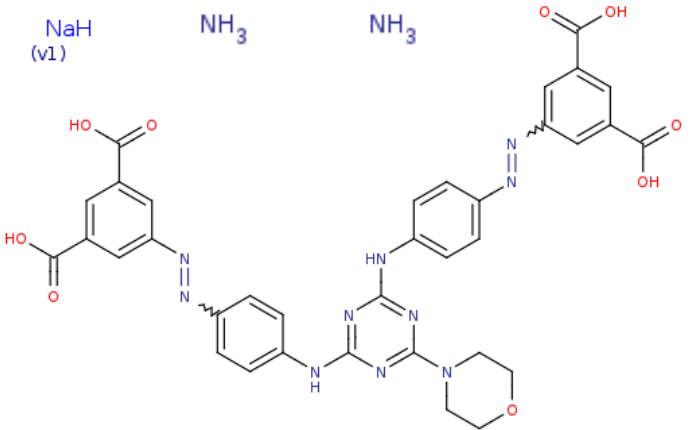
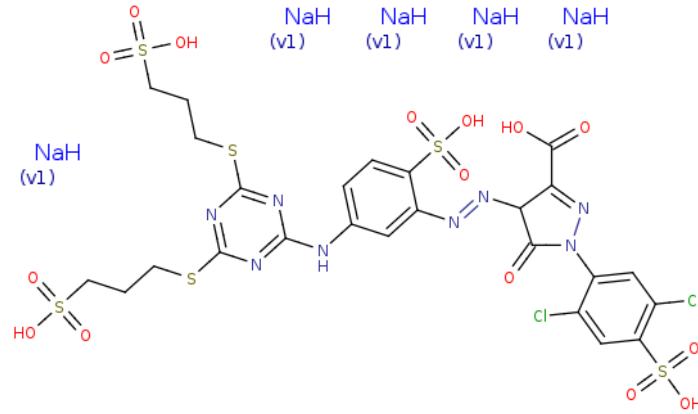
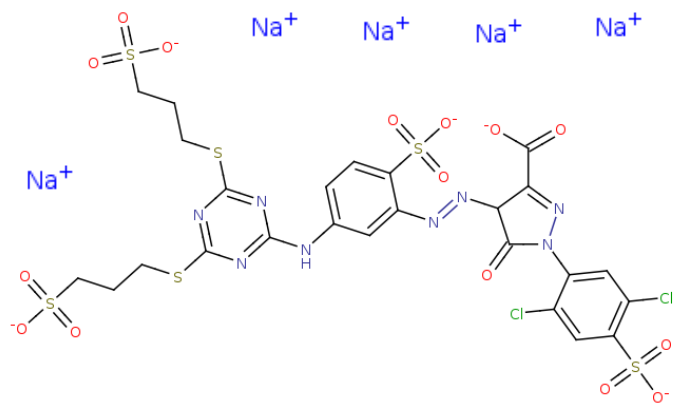
15121-89-8			EC number 438-510-4
-		Correct form in unknown. But it should be Na ⁺ instead of NaH and K ⁺ instead of KH and two H ⁺ less in the main structure	EC number 410-065-0

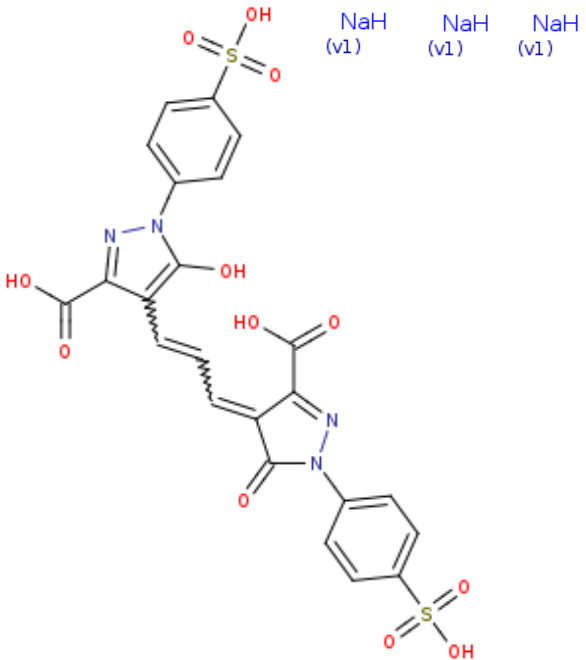
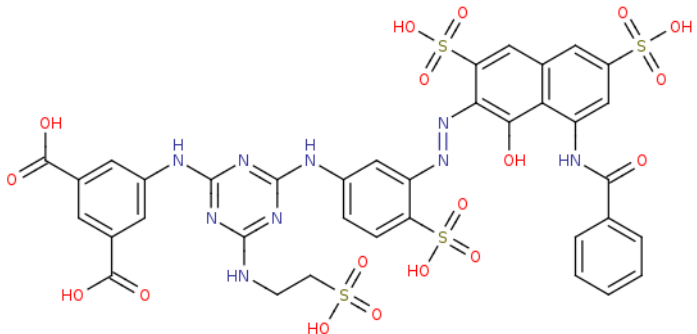
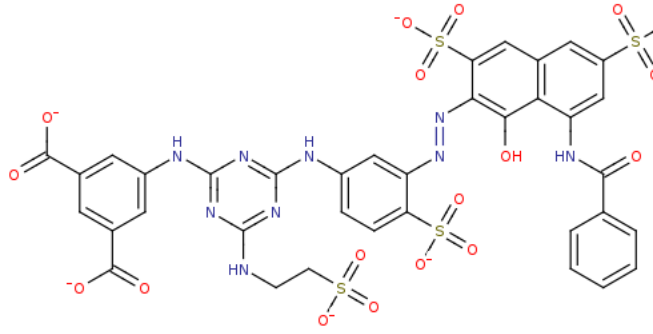
148878-21-1 (incorrect form)		EC number 412-960-1
148878-21-1 (correct form)	Correct form in unknown. But it should be Na⁺ instead of NaH and eight H⁺ less in the main structure	EC number 412-960-1
141250-43-3 (incorrect form)		EC number 435-350-7
141250-43-3 (correct form)	Correct form in unknown. But it should be Na⁺ instead of NaH and one H⁺ less in the main structure	EC number 435-350-7

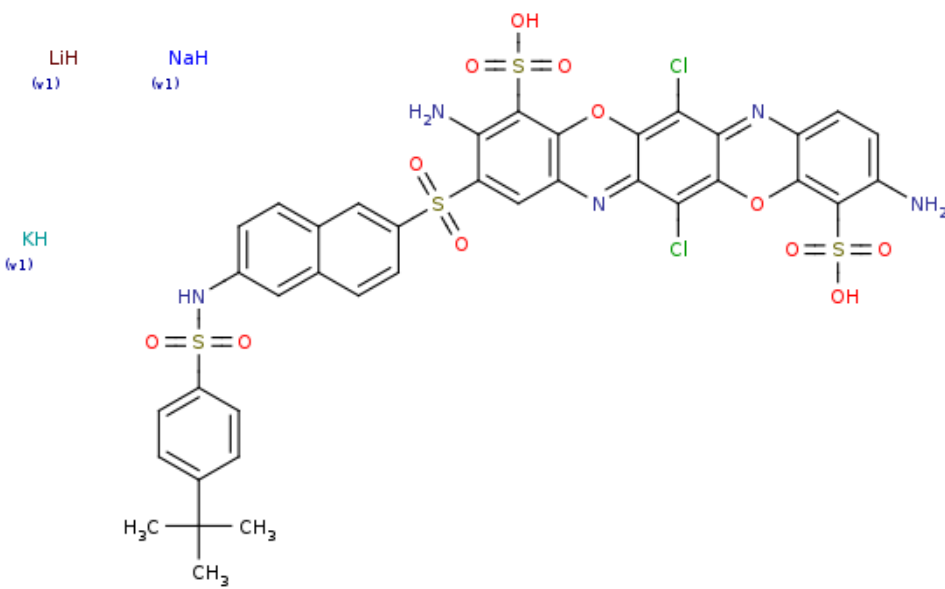
187285-15-0 (correct form)	Correct form in unknown. But it should be Na ⁺ instead of NaH and one H ⁺ less in the main structure	EC number 413-180-4
299158-63-7	NaH (v1)  Correct form in unknown. But it should be Na⁺ instead of NaH and one H⁺ less in the main structure	EC number 478-070-0
161935-19-9 (incorrect form)	NaH (v1) 	EC number 417-640-5

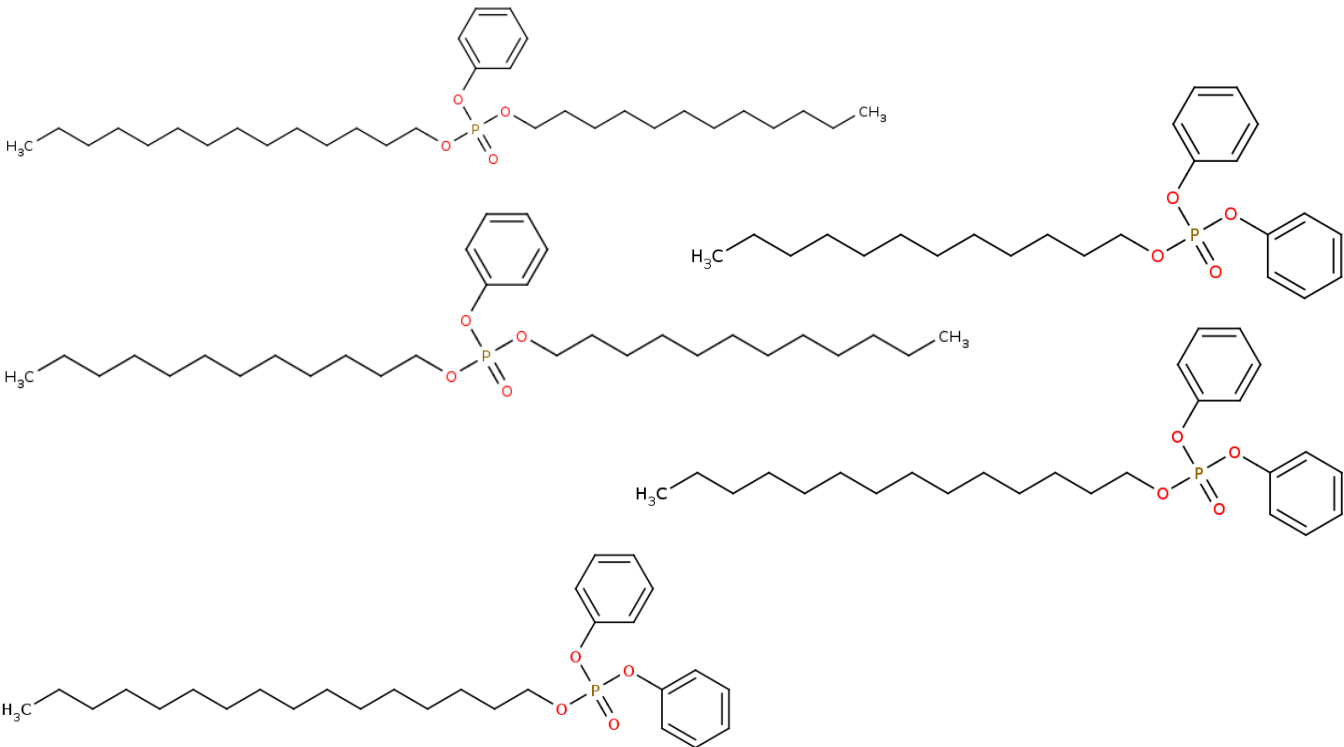
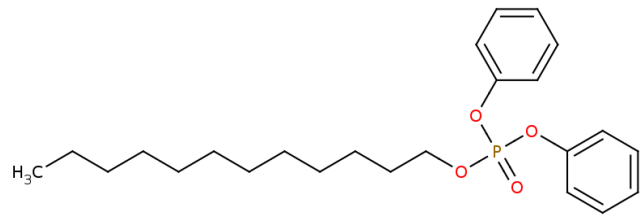
161935-19-9 (correct form)	Correct form in unknown. But it should be Na ⁺ instead of NaH and one H ⁺ less in the main structure	EC number 417-640-5
1016986-95-0		Correct form in unknown. But it should be Na ⁺ instead of NaH and Li ⁺ instead of LiH and five H ⁺ less in the main structure
		EC number 471-980-9

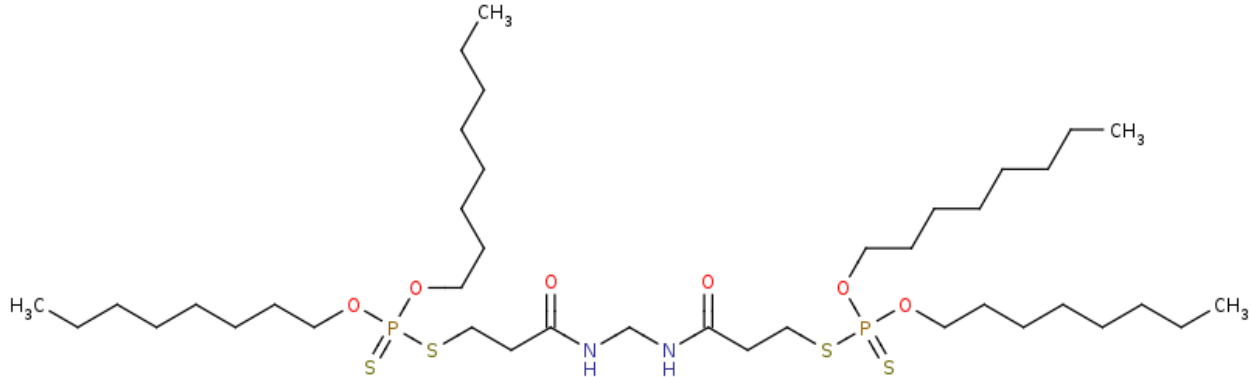
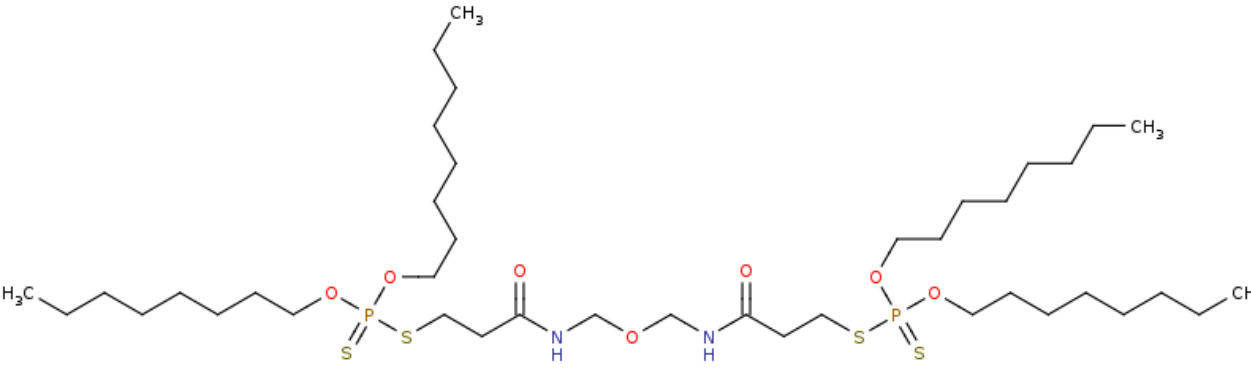
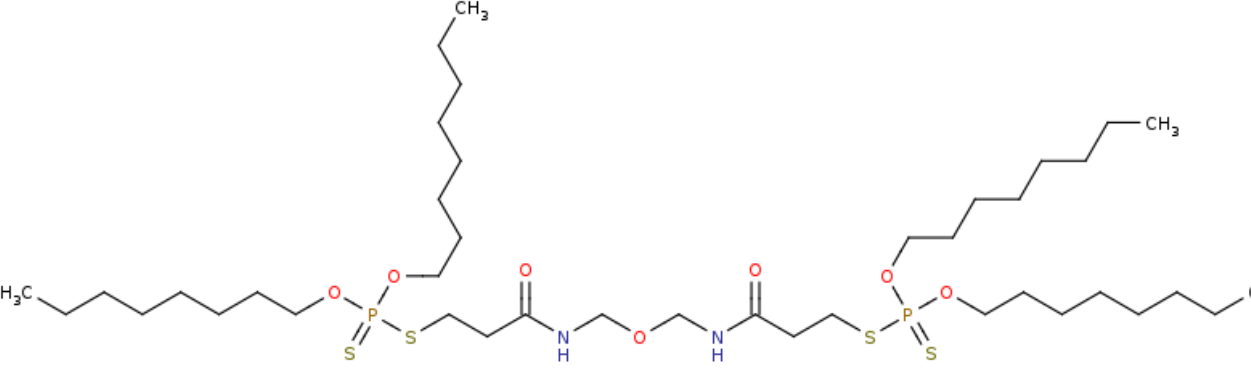
130500-97-9 (incorrect form)	 Correct form in unknown. But it should be Li+ instead of LiH and Mg2+ instead of MgH2 and four H+ less in the main structure	EC number 401-480-8	
-		Correct form in unknown. But it should be K+ instead of KH and 2 H+ less in the main structure	EC number 418-910-5

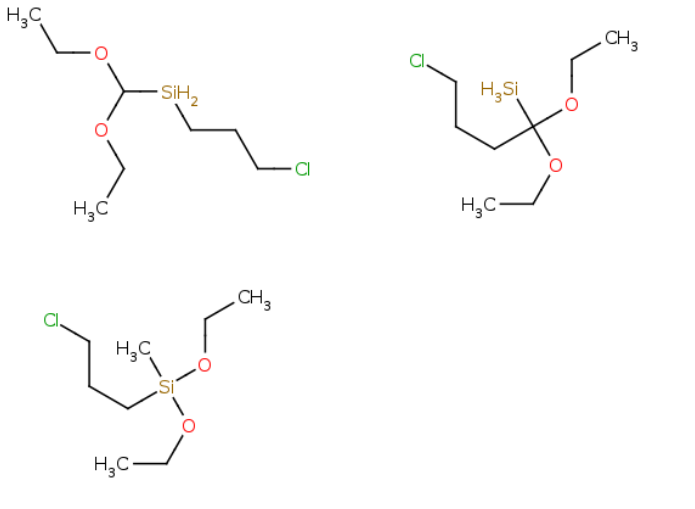
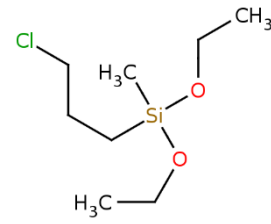
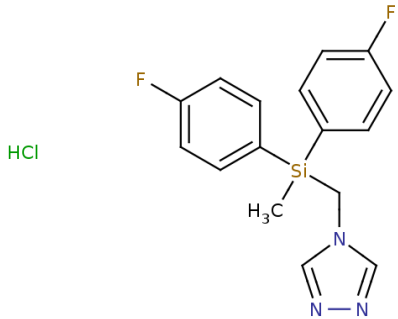
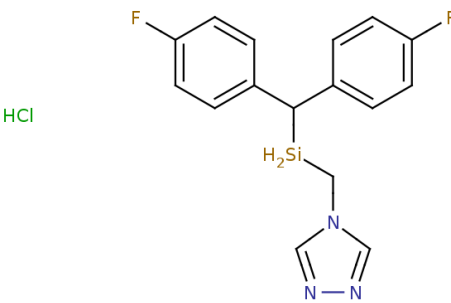
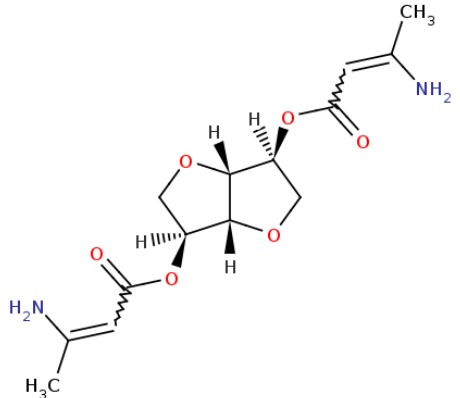
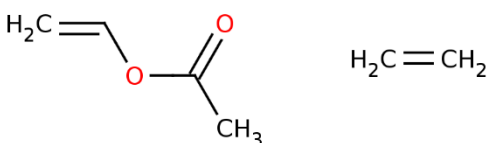
1379676-83-1		Correct form in unknown. But it should be Na⁺ instead of NaH and one H⁺ less in the main structure	EC number 414-410-6
187674-76-6			EC number 456-170-5

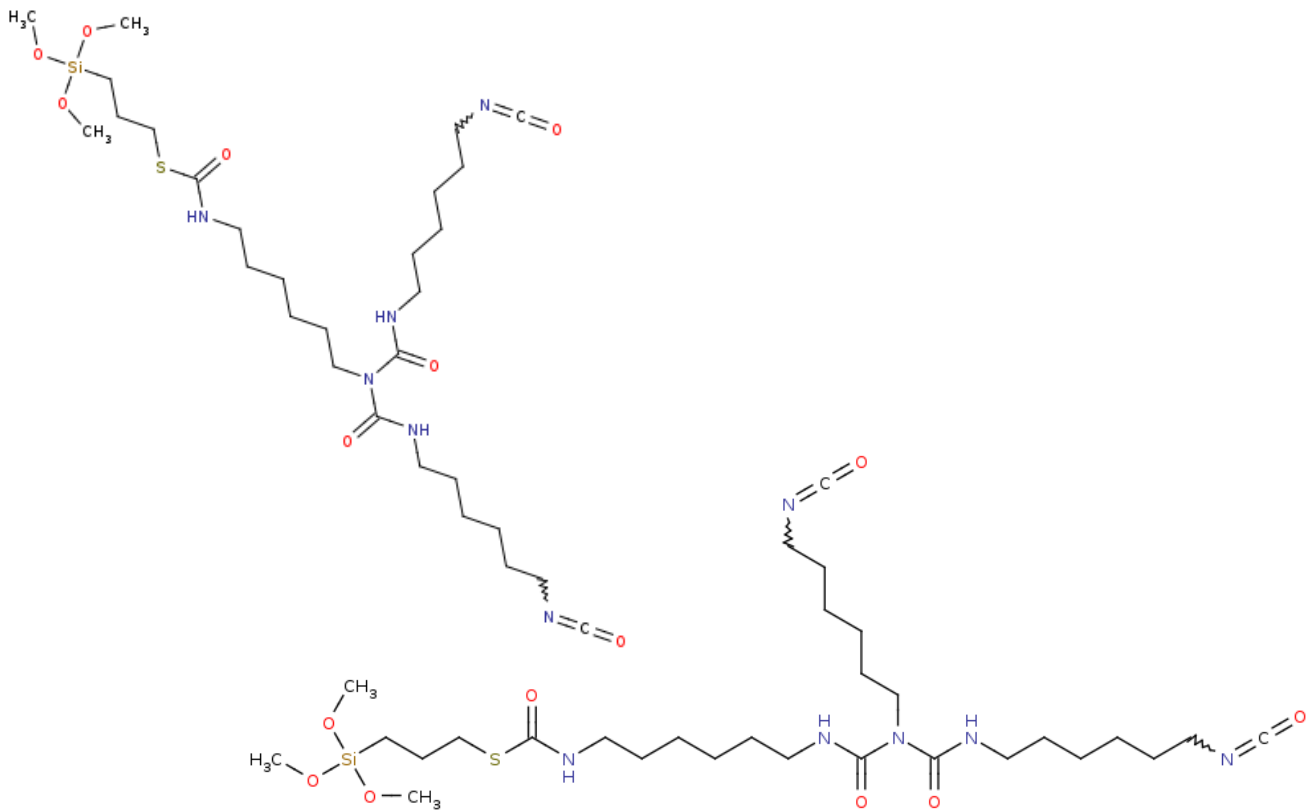
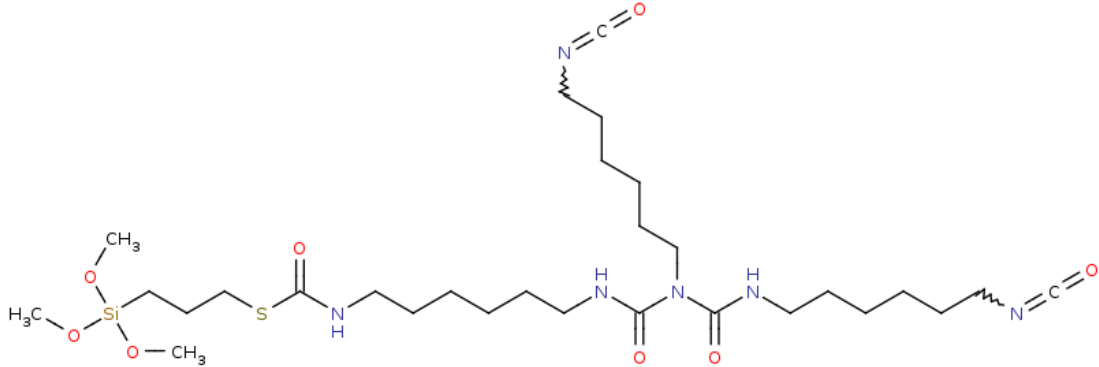
	 NaH (v1) NaH (v1) NaH (v1)	Correct form in unknown. But it should be Na⁺ instead of NaH and three H⁺ less in the main structure	EC number 426-690-7
	 NaH (v1) NaH (v1) NaH (v1) NaH (v1) NaH (v1) NaH (v1)	 Na⁺ Na⁺ Na⁺ Na⁺ Na⁺ Na⁺	EC number 482-150-0

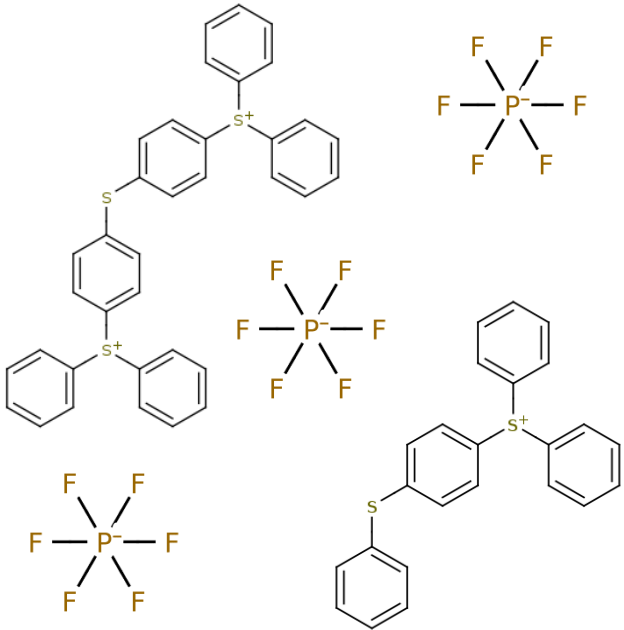
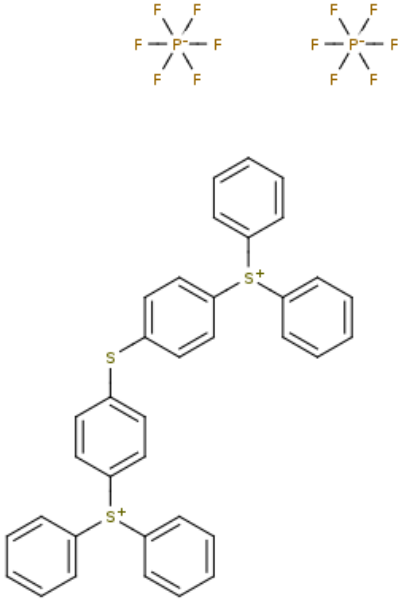
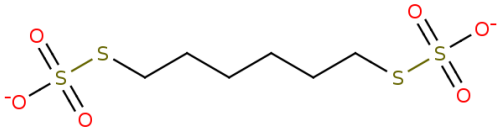
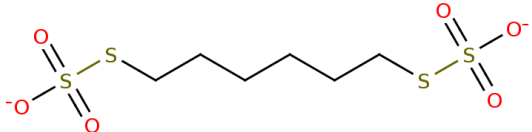
371921-63-0 (incorrect form)		EC number 440-770-9
371921-63-0 (correct form)	Correct form in unknown. But it should be Na⁺ instead of NaH, K⁺ instead of KH, and Li⁺ instead of LiH and three H⁺ less in the main structure	

27460-02-2 (incorrect form)		EC number 431-760-5
27460-02-2 (correct form)		EC number 431-760-5 CAS contains only one of the structures

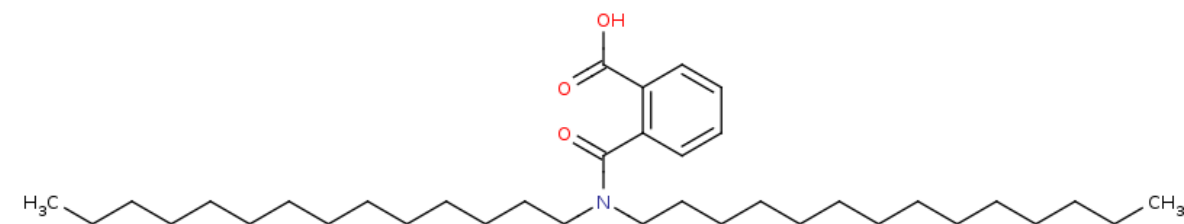
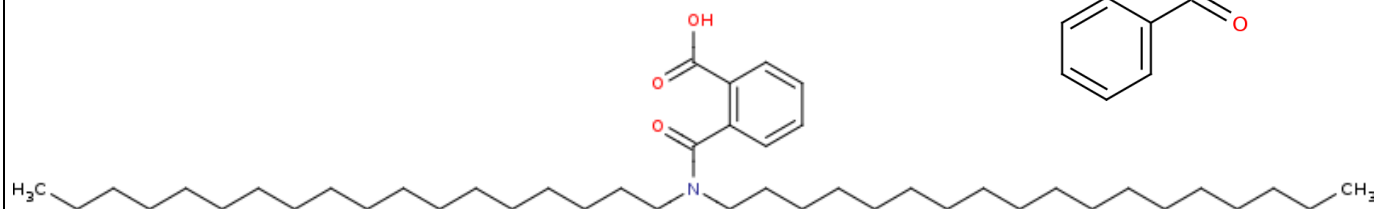
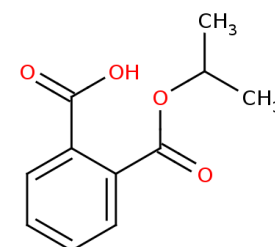
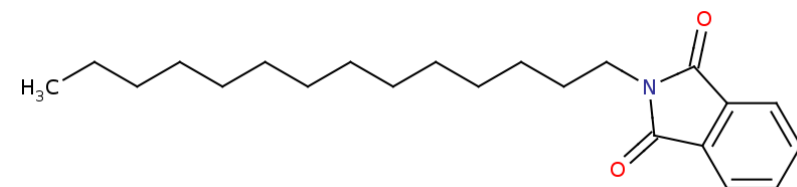
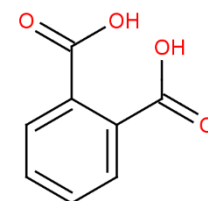
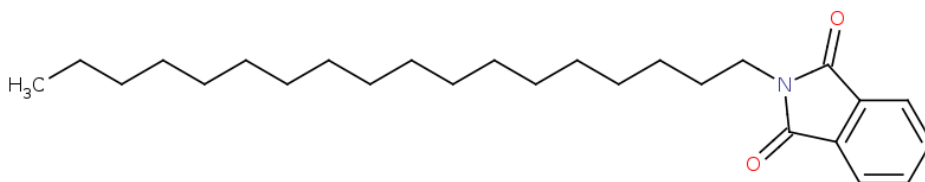
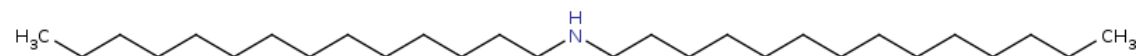
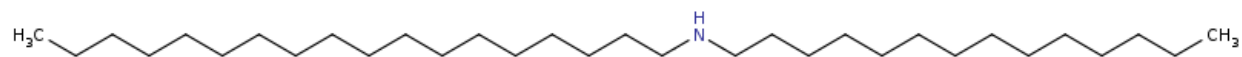
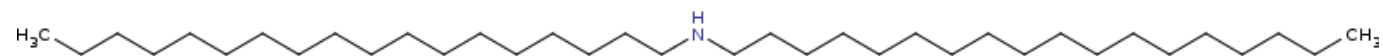
793710-14-2 (incorrect form)	 	EC number 401-820-5
793710-14-2 (correct form)		EC number 401-820-5 CAS RN™ contains only the second structure

13501-76-3			EC number 236-828-6 CAS RN™ contains only the third structure
89066-61-5			EC number 401-380-4
24937-78-8			EC number 429-840-1

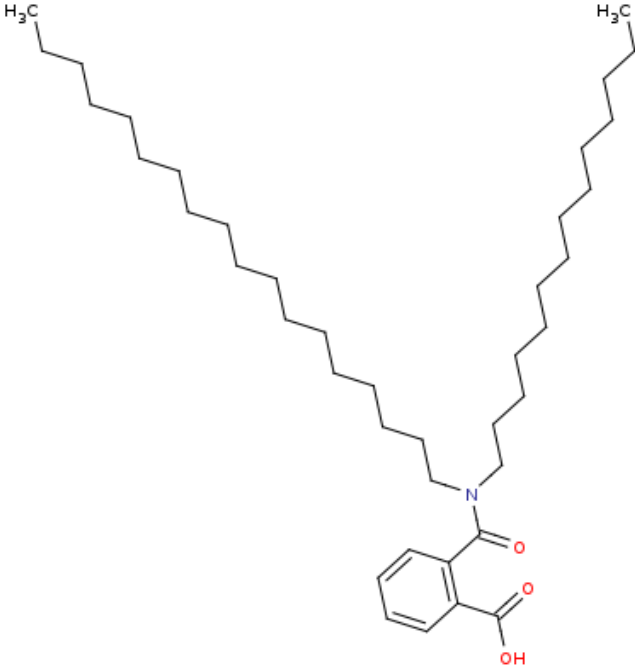
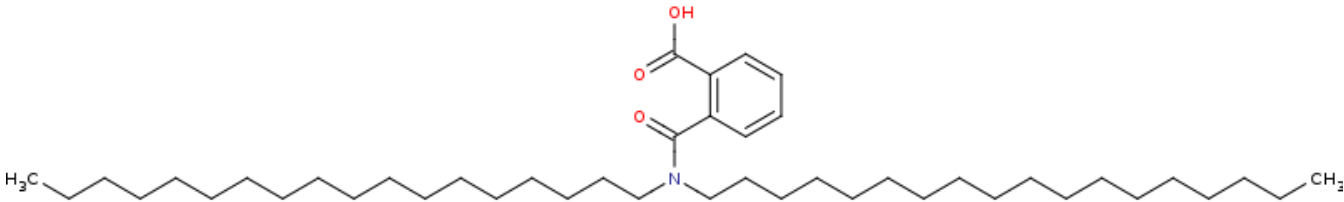
85702-90-5 (incorrect form)		EC number 402-290-8
85702-90-5 (correct form)		EC number 402-290-8 CAS RN™ contains only the second structure

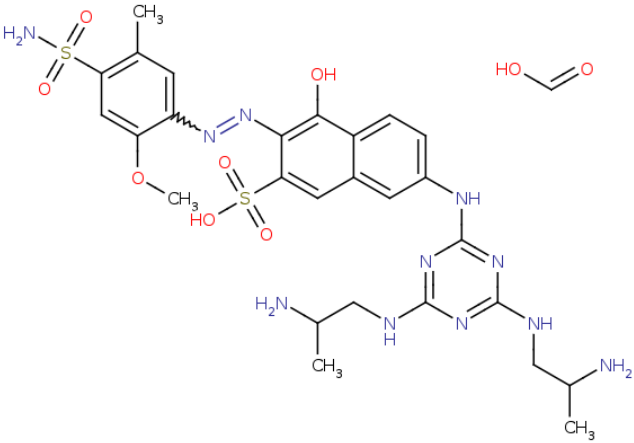
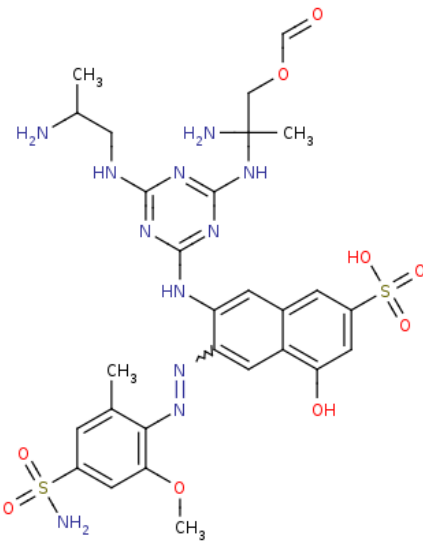
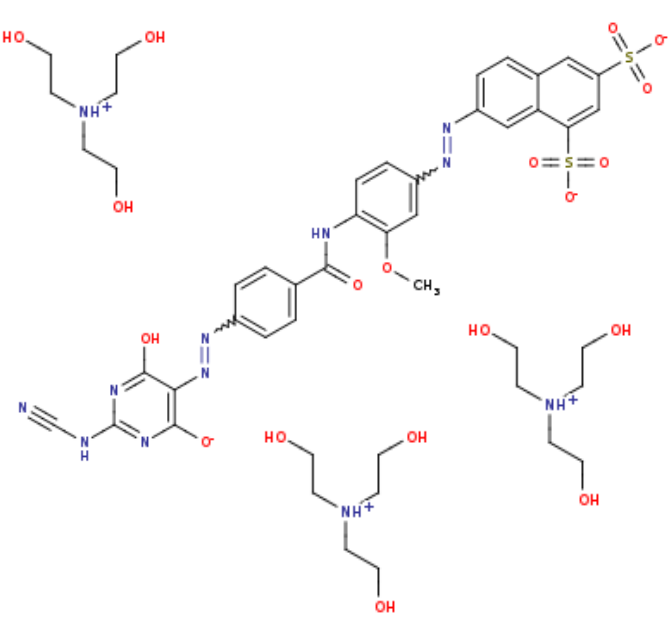
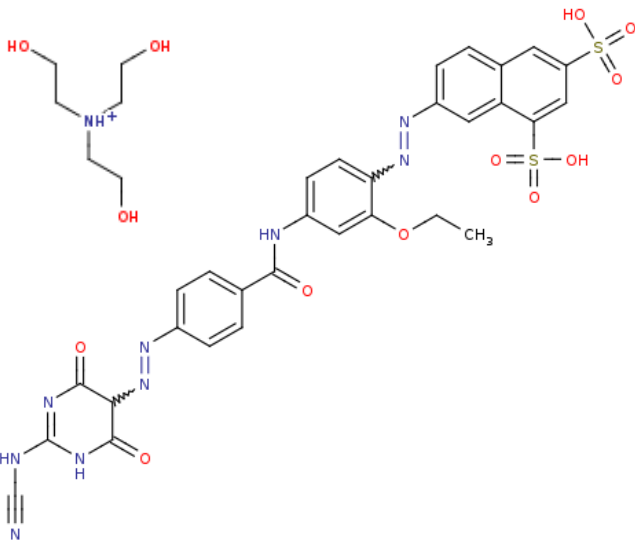
74227-35-3			EC number 404-986-7 CAS RN™ does not contain all structural elements
5719-73-3	H_2O H_2O Na^+ Na^+ 	Na^+ Na^+ 	EC number 401-320-7

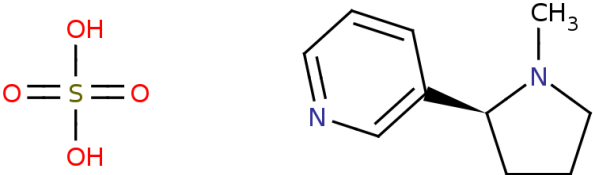
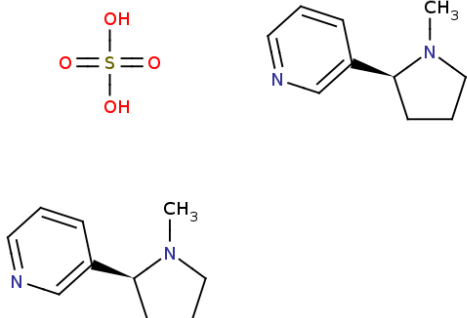
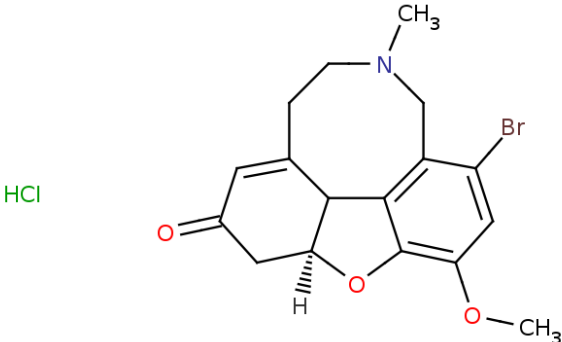
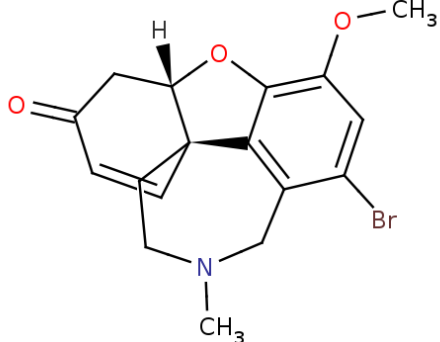
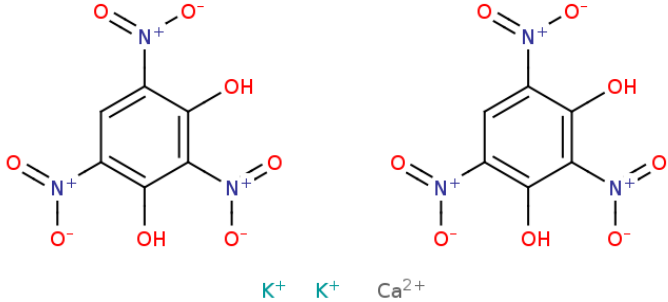
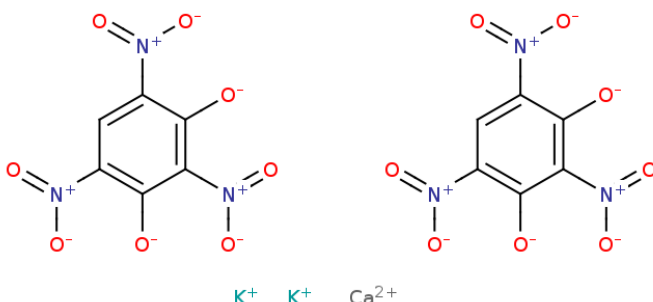
87787-81-3
(incorrect
from part 1)

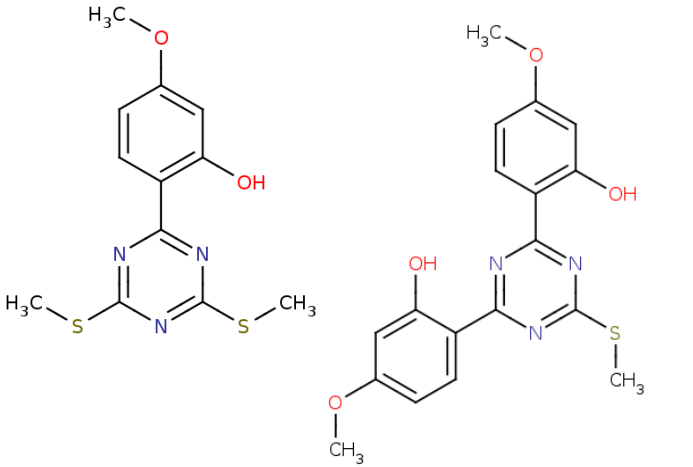
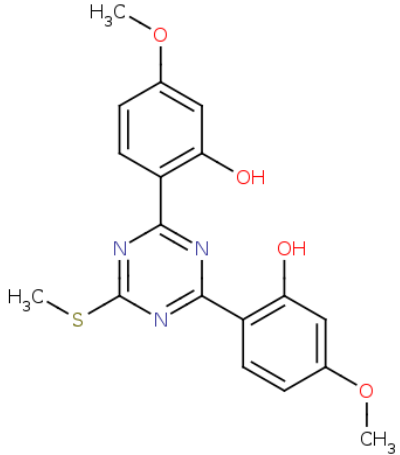
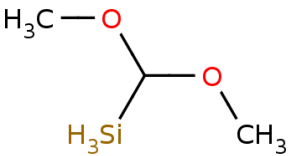
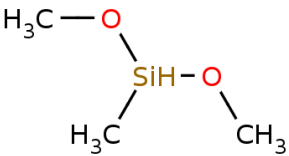
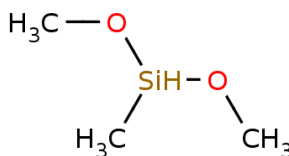
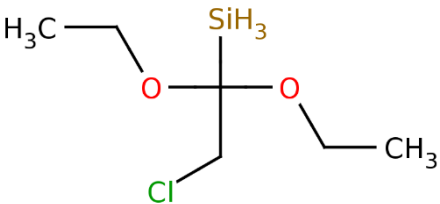
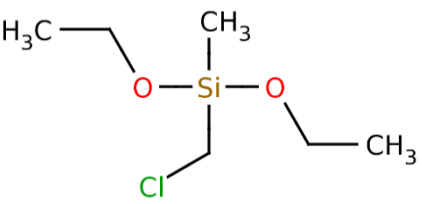


EC number
413-800-3

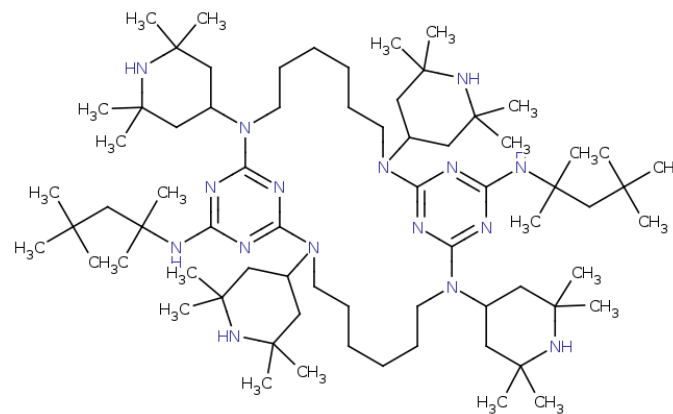
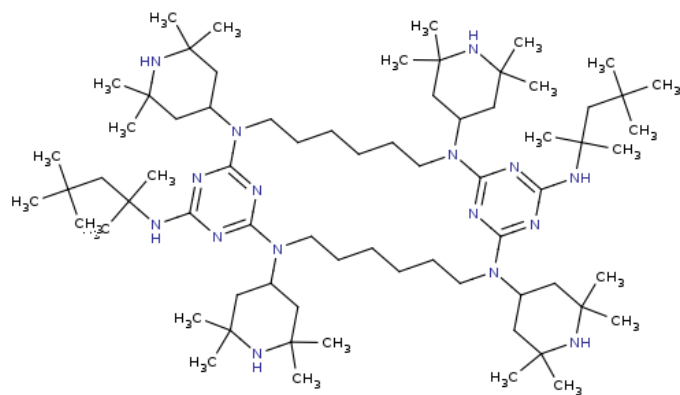
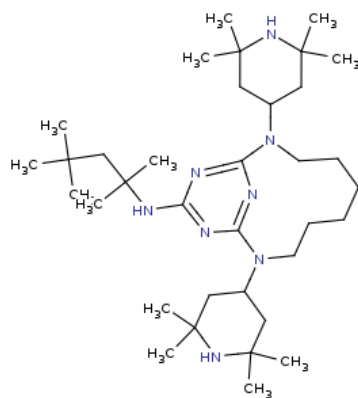
87787-81-3 (incorrect from part 2)		EC number 413-800-3
87787-81-3 (correct from)		EC number 413-800-3 CAS does not contain all structural elements

784157-49-9			EC number 424-260-3
778583-04-3			EC number 421-440-3

65-30-5			EC number 200-606-7
183487-56-1			EC number 439-750-2 CAS RN™ is not with HCl
1265906-36-2			EC number 825-439-2

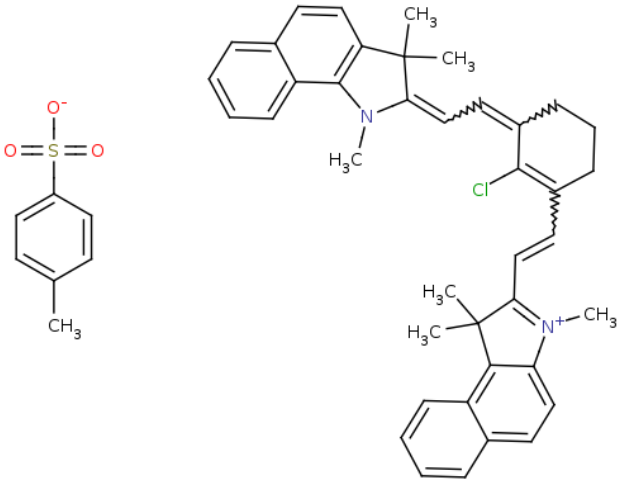
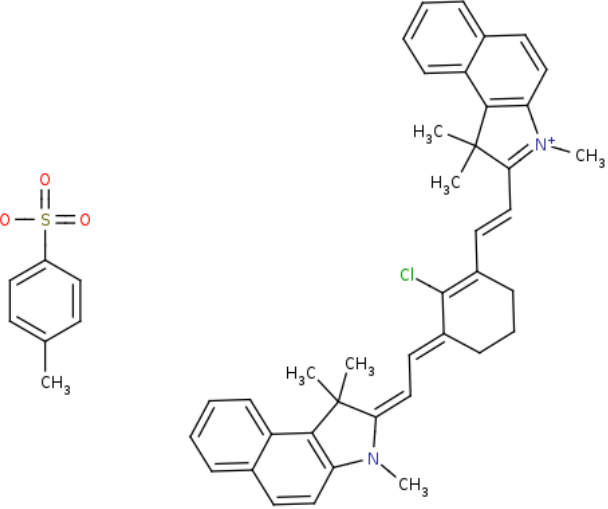
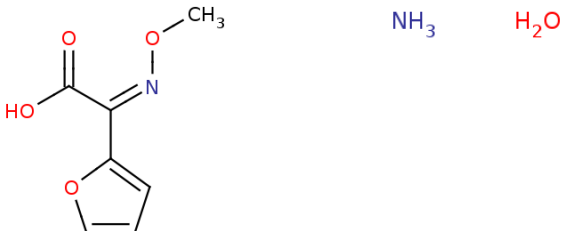
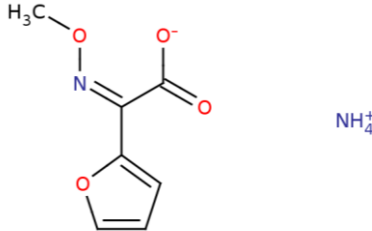
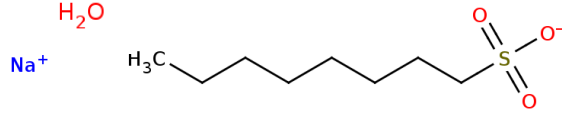
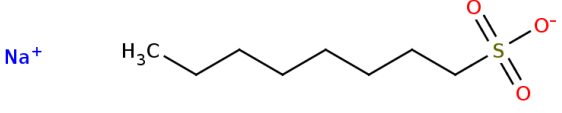
156137-33-6	 Chemical structure of 1,3-bis(methylthio)-5-methoxy-2-((4-methoxyphenyl)thio)-1,2,4-triazine. The structure features a 1,2,4-triazine ring substituted with two methylthio groups at positions 1 and 3, a methoxy group at position 5, and a (4-methoxyphenyl)thio group at position 2.	 Chemical structure of 1,3-bis(methylthio)-5-methoxy-2-((4-methoxyphenyl)thio)-1,2,4-triazine. The structure features a 1,2,4-triazine ring substituted with two methylthio groups at positions 1 and 3, a methoxy group at position 5, and a (4-methoxyphenyl)thio group at position 2.	EC number 423-520-3 CAS contains only the second structure
16881-77-9	 Chemical structure of dimethylsilane (H₃Si-CH₃).  Chemical structure of dimethylsilane (H₃Si-CH₃).	 Chemical structure of dimethylsilane (H₃Si-CH₃).	EC number 240-914-9
2212-10-4	 Chemical structure of 1-chloro-2-ethoxy-2-(chloromethyl)ethylsilane. The structure features a central silicon atom bonded to a methyl group, a hydrogen atom, and two ethoxy groups, with a chlorine atom attached to the central carbon.	 Chemical structure of 1-chloro-2-ethoxy-2-(chloromethyl)ethylsilane. The structure features a central silicon atom bonded to a methyl group, a hydrogen atom, and two ethoxy groups, with a chlorine atom attached to the central carbon.	EC number 218-657-9

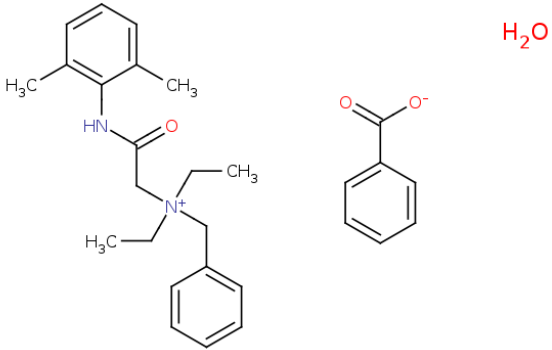
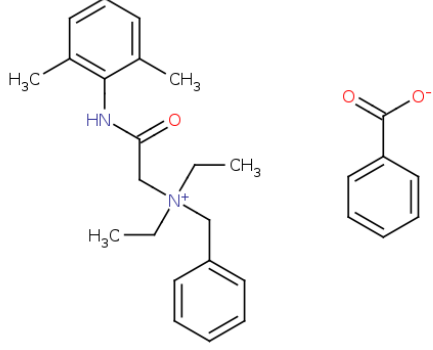
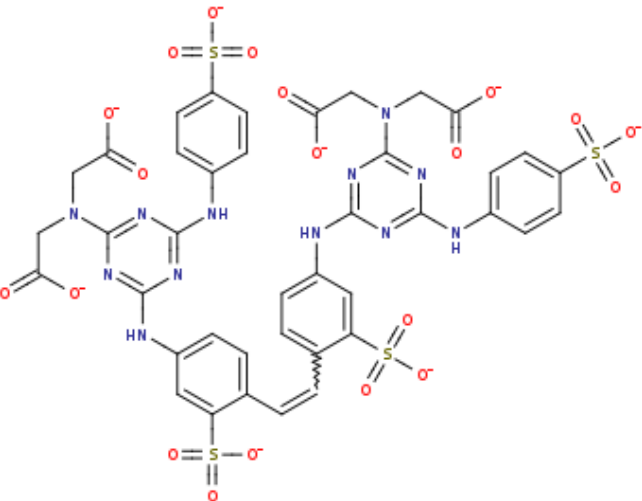
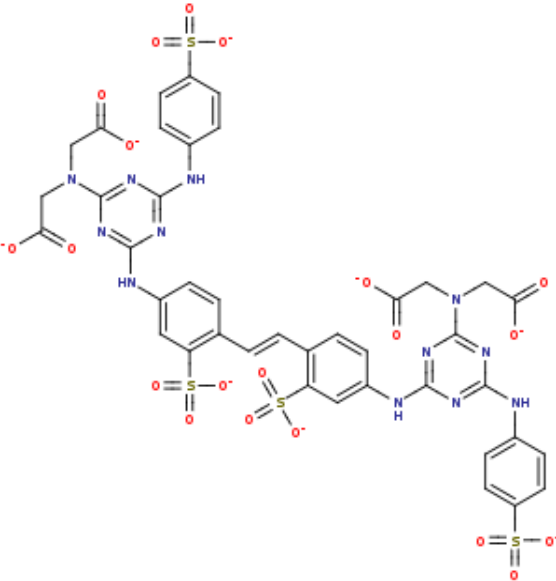
86168-95-8

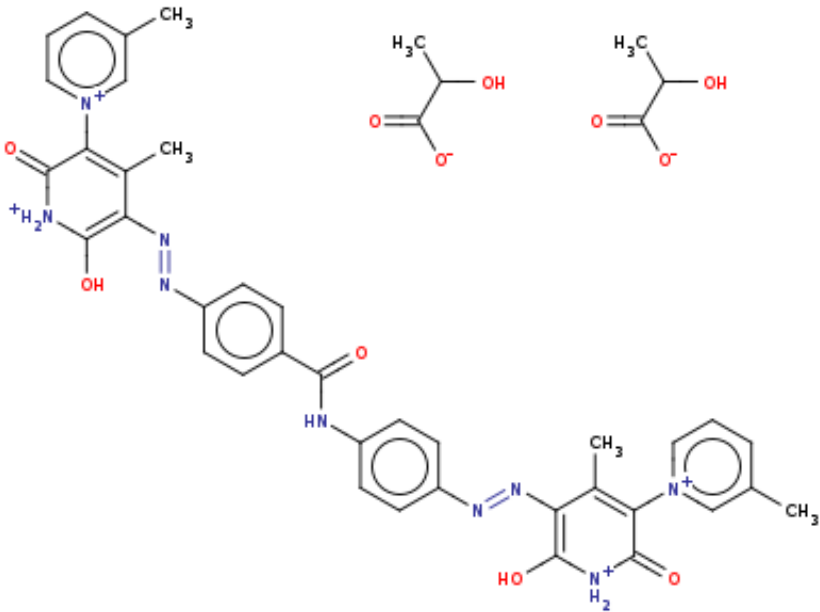
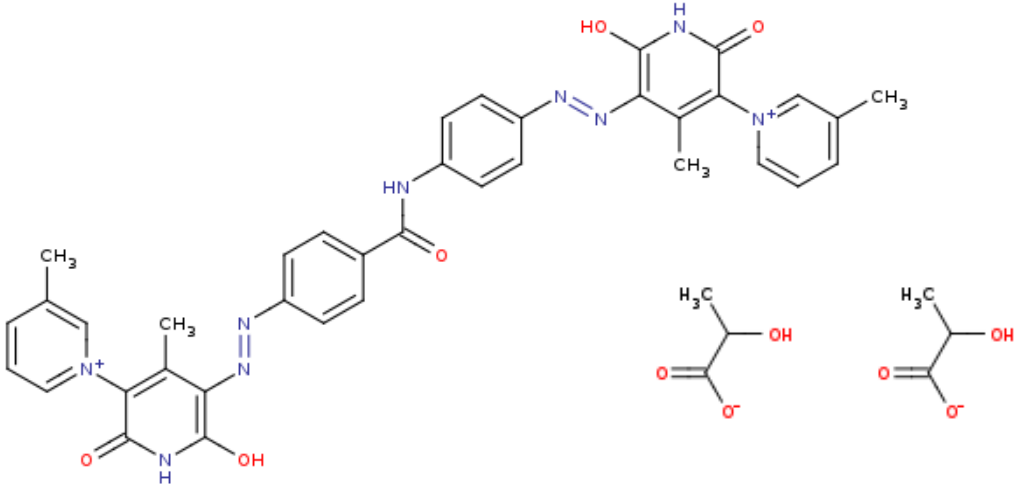


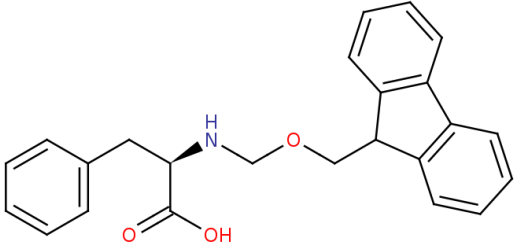
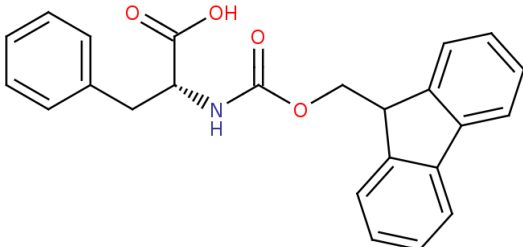
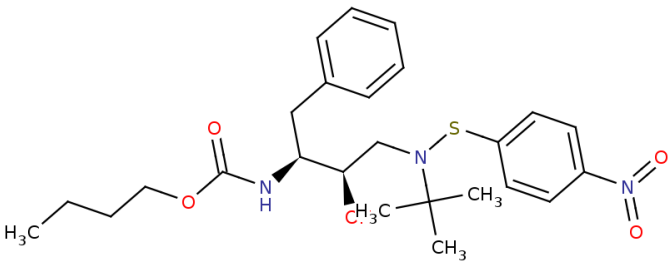
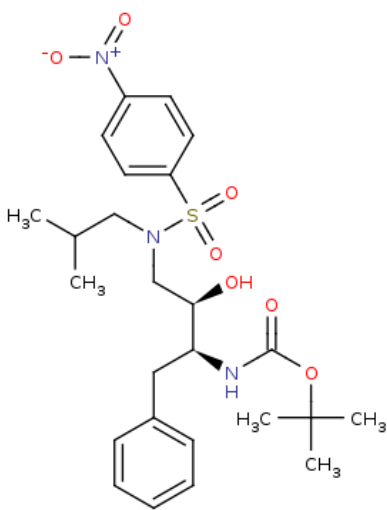
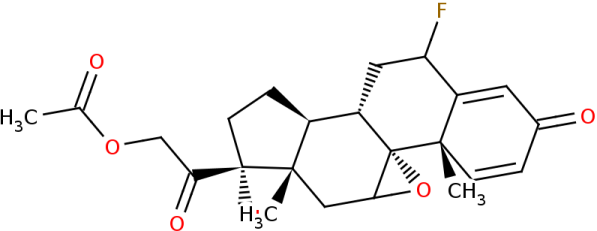
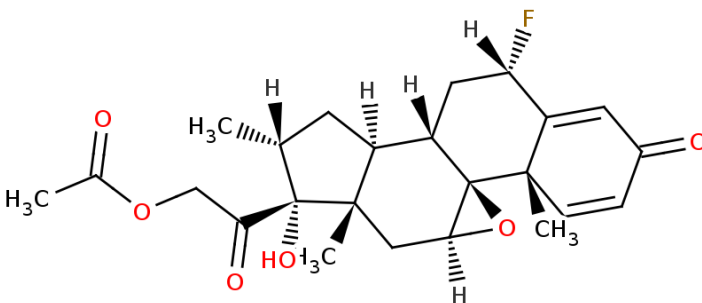
EC number
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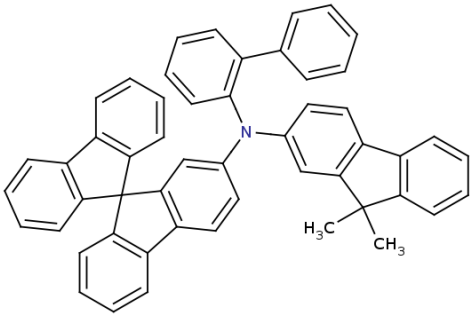
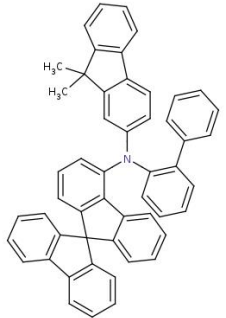
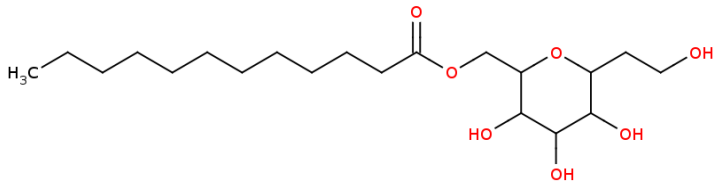
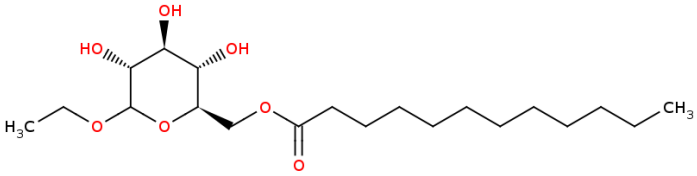
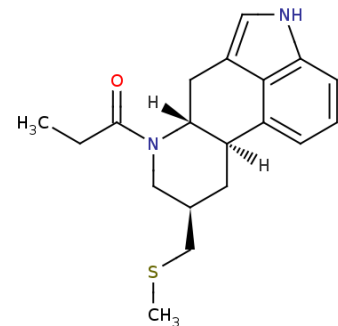
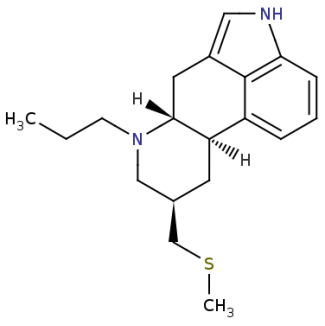
CAS contains
only the
second
structure

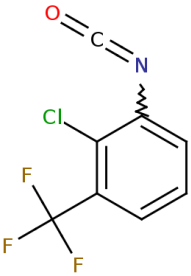
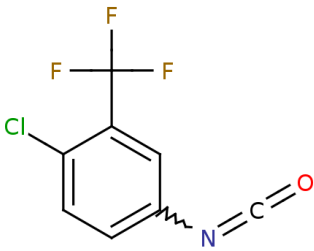
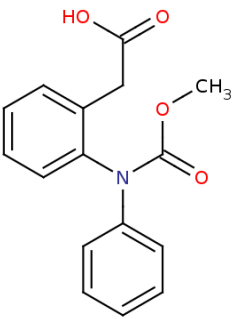
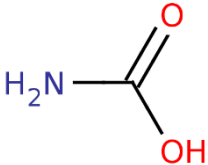
134127-48-3			EC number 420-680-6
97148-39-5			EC number 405-990-1 additional water that is not in the CAS registration
5324-84-5	 additional water that is not in the CAS registration		EC number 226-195-4

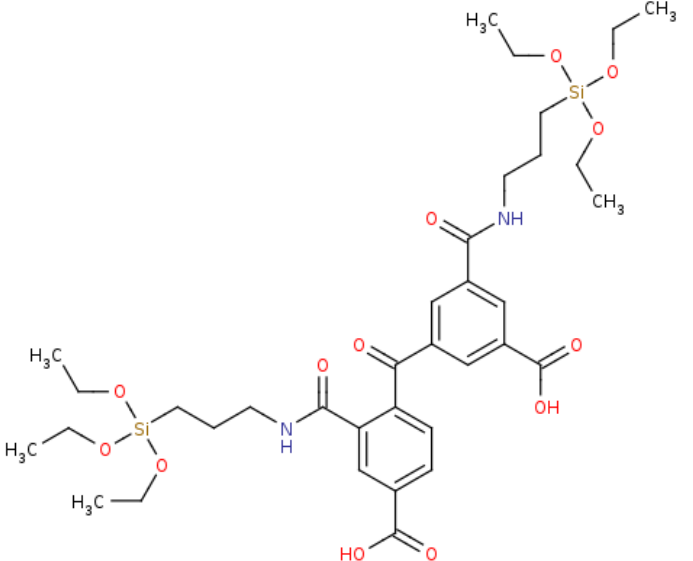
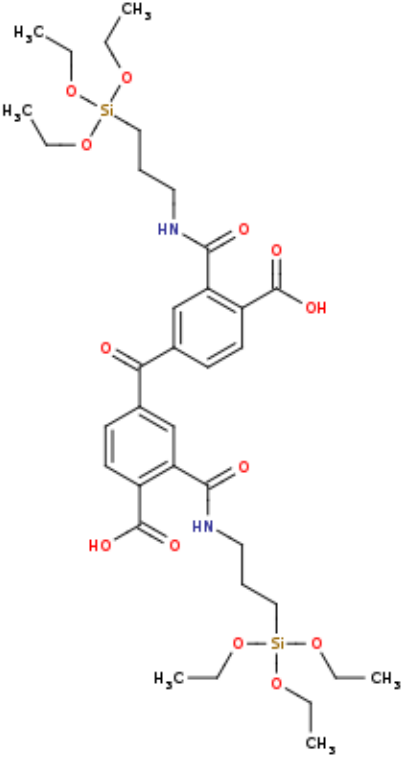
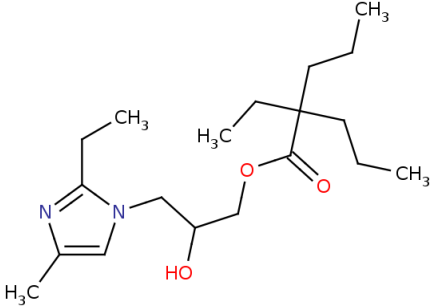
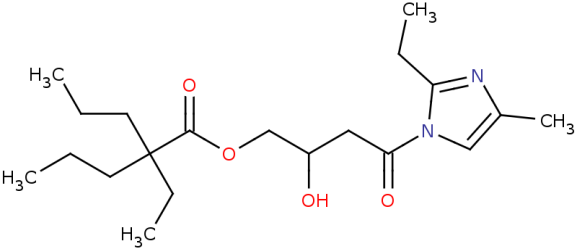
3734-33-6	 Chemical structure of 2,6-dimethyl-N-((2-ethyl-1-phenylethyl)carbamoyl)aniline and benzoate ion, with H_2O.	 Chemical structure of 2,6-dimethyl-N-((2-ethyl-1-phenylethyl)carbamoyl)aniline and benzoate ion.	EC number 223-095-2 additional water that is not in the CAS registration
174305-36-3	 Chemical structure of a complex sulfonated nucleoside derivative, with H_2O and Na^+ ions.	 Chemical structure of a complex sulfonated nucleoside derivative, with Na^+ ions.	EC number 416-640-2 additional water that is not in the CAS registration

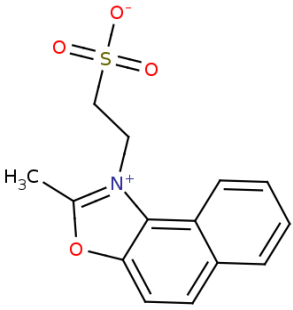
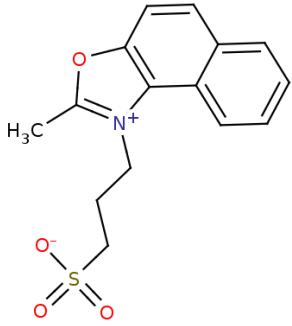
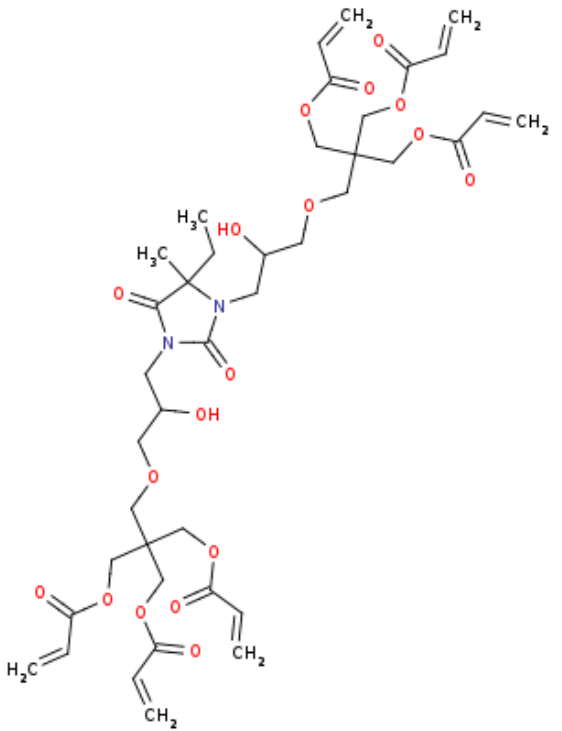
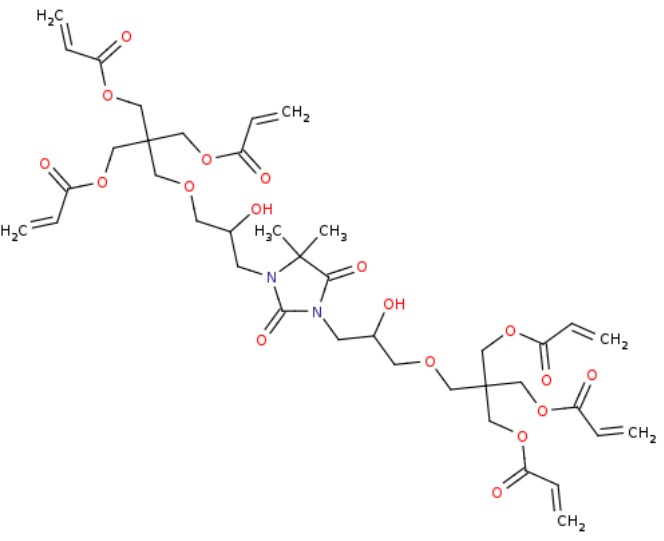
75214-63-0 (incorrect form)	 The structure shows a complex molecule with two pyridinium rings. The left pyridinium ring is substituted with a methyl group at the 3-position and a hydroxyl group at the 4-position. It is connected via an azo group to a central benzene ring, which is further connected to another pyridinium ring substituted with a methyl group at the 3-position and a hydroxyl group at the 4-position. Two lactic acid molecules are shown as separate entities.	EC number 278-130-4
75214-63-0 (correct form)	 The structure shows a complex molecule with two pyridinium rings. The left pyridinium ring is substituted with a methyl group at the 3-position and a hydroxyl group at the 4-position. It is connected via an azo group to a central benzene ring, which is further connected to another pyridinium ring substituted with a methyl group at the 3-position and a hydroxyl group at the 4-position. Two lactic acid molecules are shown as separate entities.	EC number 278-130-4

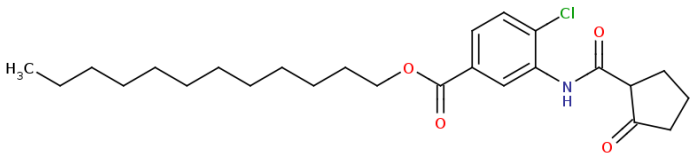
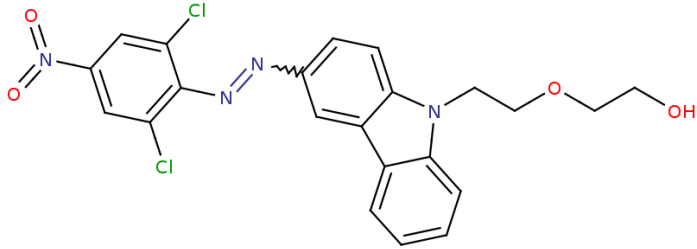
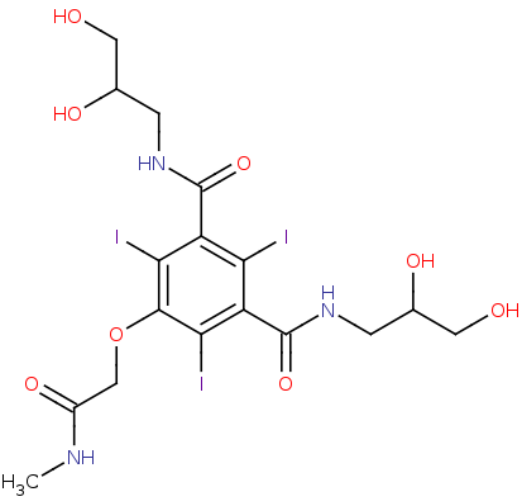
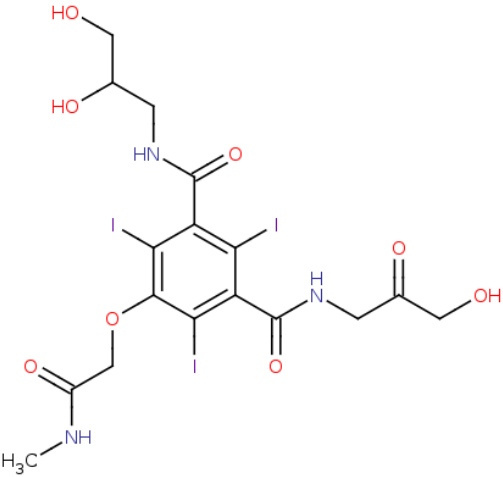
86123-10-6	 Chemical structure of (S)-1-(benzyloxy)-2-phenylpropan-1-ol-1-ol. It features a central carbon atom bonded to a hydroxyl group (red), a benzyl group (phenyl ring attached to a CH2 group), a benzyloxy group (benzyl group attached to an oxygen atom), and a hydrogen atom (not shown).	 Chemical structure of (S)-1-(benzyloxy)-2-phenylpropan-1-ol-1-ol. It features a central carbon atom bonded to a hydroxyl group (red), a benzyl group (phenyl ring attached to a CH2 group), a benzyloxy group (benzyl group attached to an oxygen atom), and a hydrogen atom (not shown).	EC number 440-090-2
191226-98-9	 Chemical structure of (S)-1-(benzyloxy)-2-phenylpropan-1-ol-1-ol. It features a central carbon atom bonded to a hydroxyl group (red), a benzyl group (phenyl ring attached to a CH2 group), a benzyloxy group (benzyl group attached to an oxygen atom), and a hydrogen atom (not shown).	 Chemical structure of (S)-1-(benzyloxy)-2-phenylpropan-1-ol-1-ol. It features a central carbon atom bonded to a hydroxyl group (red), a benzyl group (phenyl ring attached to a CH2 group), a benzyloxy group (benzyl group attached to an oxygen atom), and a hydrogen atom (not shown).	EC number 467-070-6
4571-51-1	 Chemical structure of (S)-1-(benzyloxy)-2-phenylpropan-1-ol-1-ol. It features a central carbon atom bonded to a hydroxyl group (red), a benzyl group (phenyl ring attached to a CH2 group), a benzyloxy group (benzyl group attached to an oxygen atom), and a hydrogen atom (not shown).	 Chemical structure of (S)-1-(benzyloxy)-2-phenylpropan-1-ol-1-ol. It features a central carbon atom bonded to a hydroxyl group (red), a benzyl group (phenyl ring attached to a CH2 group), a benzyloxy group (benzyl group attached to an oxygen atom), and a hydrogen atom (not shown).	EC number 941-489-9

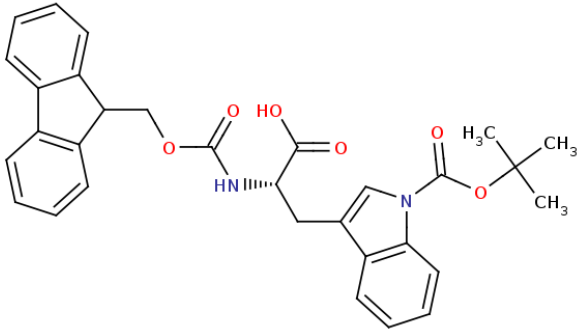
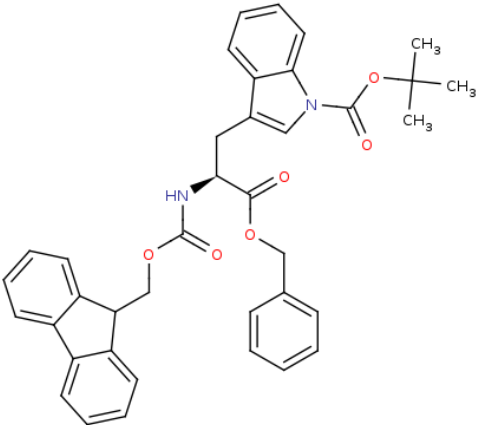
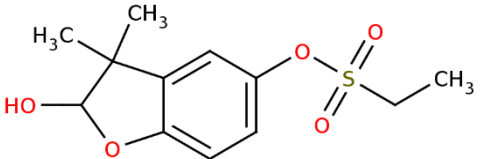
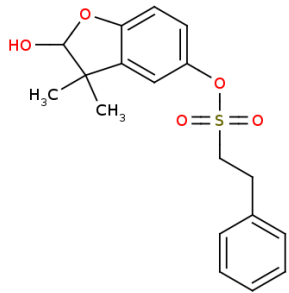
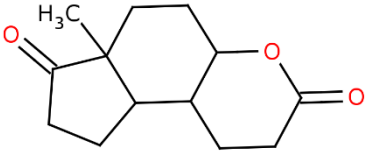
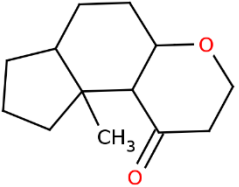
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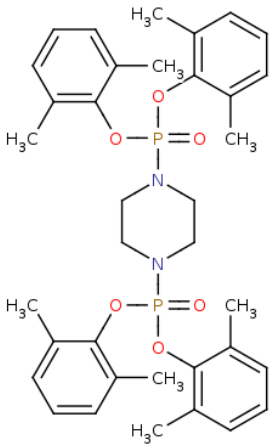
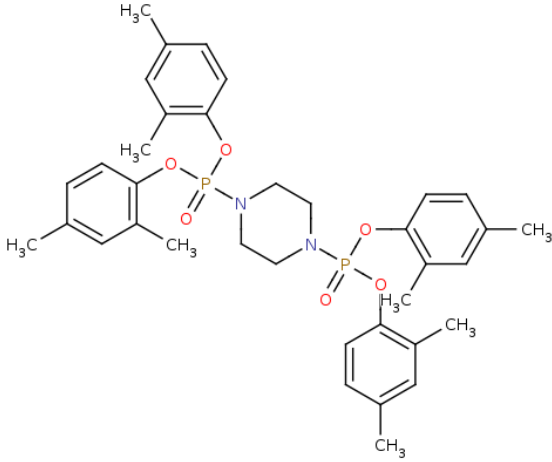
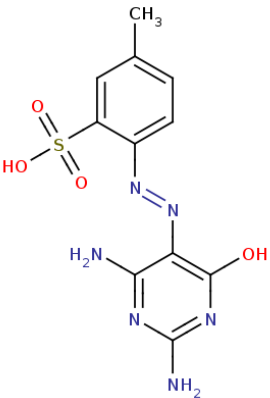
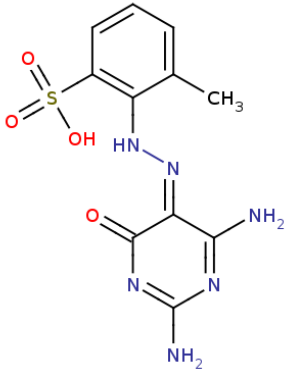
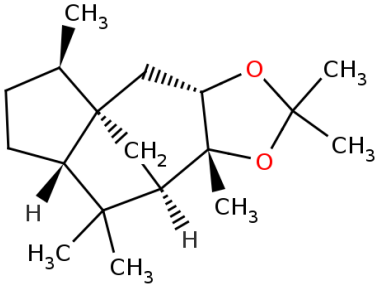
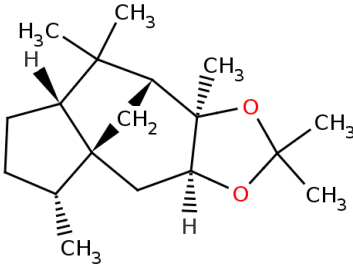
327-78-6	 Chemical structure of 1-(2-chloro-4-(trifluoromethyl)phenyl)isocyanide. It features a benzene ring with a chlorine atom at the 2-position and a trifluoromethyl group at the 4-position. An isocyanide group (-N=C=O) is attached to the 1-position of the ring.	 Chemical structure of 1-(2-chloro-4-(trifluoromethyl)phenyl)isocyanide. It features a benzene ring with a chlorine atom at the 2-position and a trifluoromethyl group at the 4-position. An isocyanide group (-N=C=O) is attached to the 1-position of the ring.	EC number 455-070-9
463-77-4	 Chemical structure of N-(2-(2-oxo-2-(phenylamino)ethyl)phenyl)benzamide. It consists of a central benzene ring with a carboxylic acid group (-COOH) at the 1-position and a benzamide group (-NHC(=O)Ph) at the 2-position. The benzamide group is further substituted with a phenyl ring.	 Chemical structure of Glycine. It consists of a central carbon atom bonded to an amino group (-NH₂), a carboxylic acid group (-COOH), and two hydrogen atoms.	EC number 439-530-6

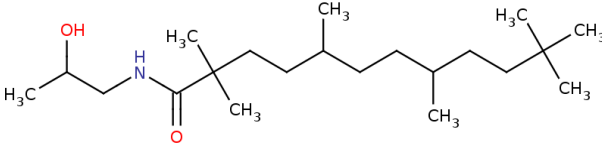
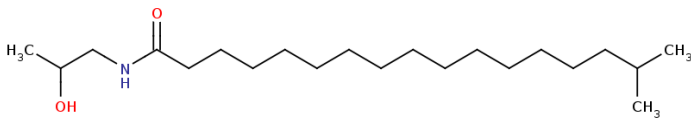
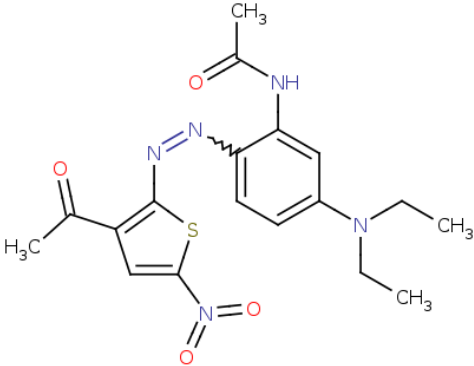
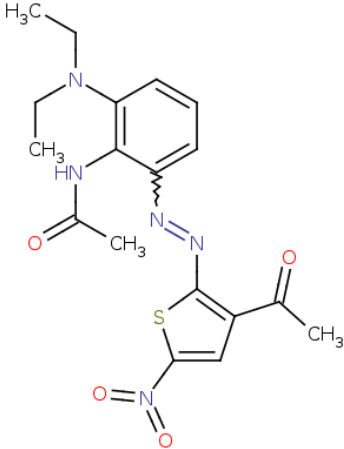
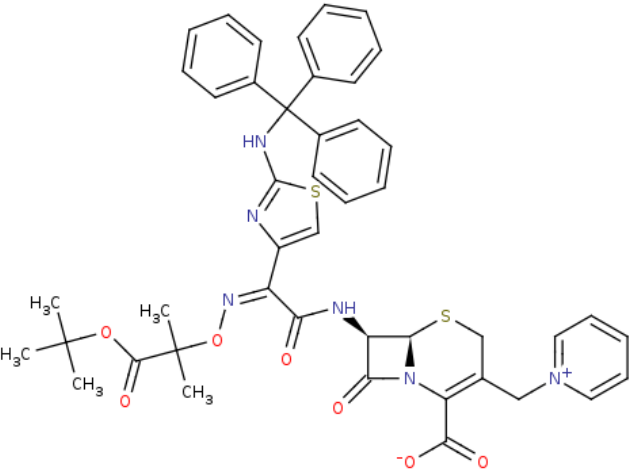
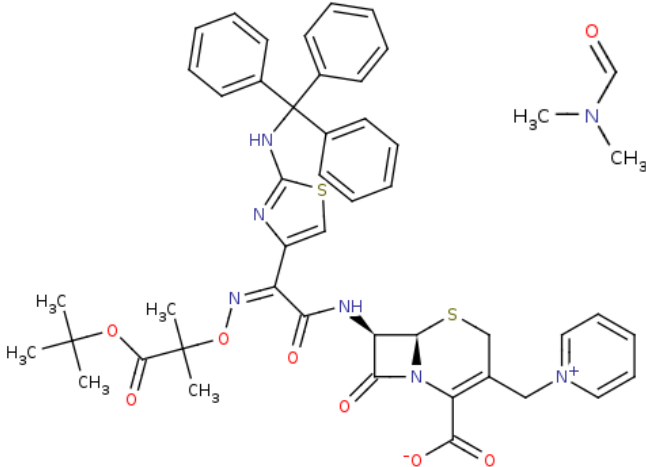
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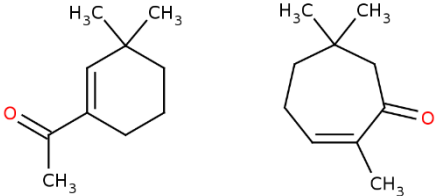
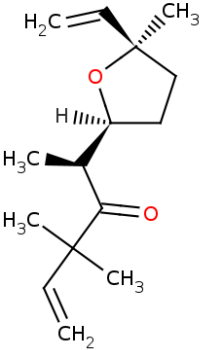
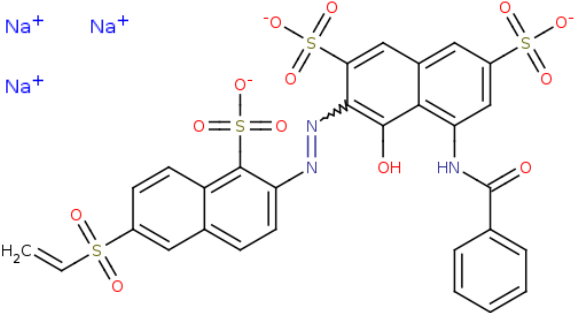
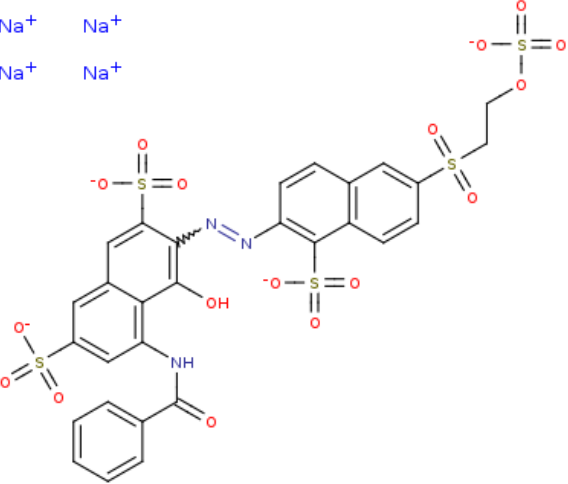
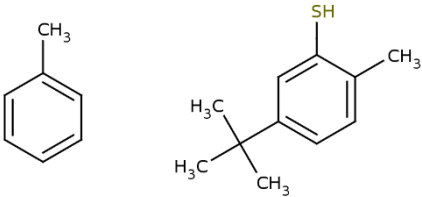
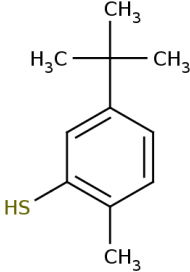
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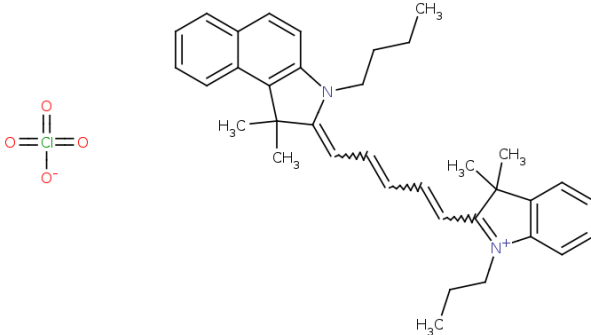
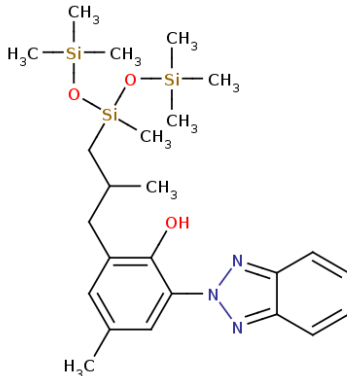
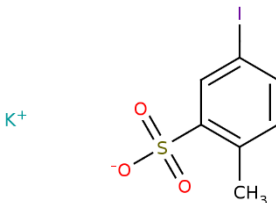
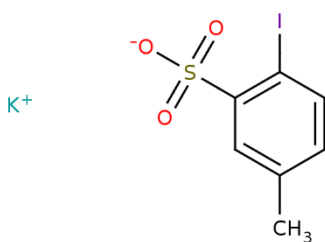
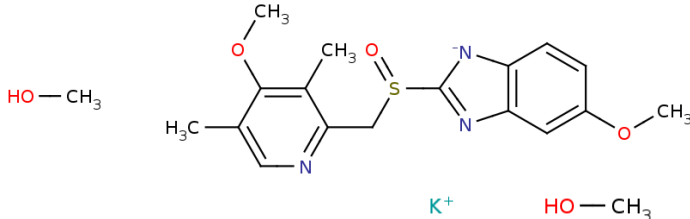
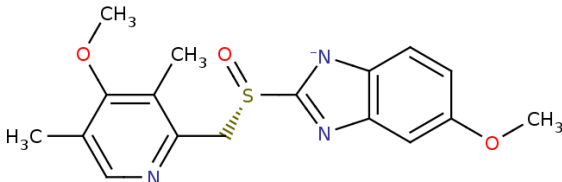
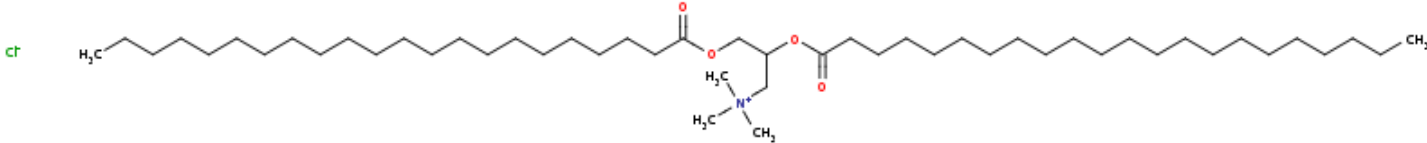
2135870-35-6	 Chemical structure of 1-(2-chloro-4-((9-oxocyclopentylideneamino)oxy)phenyl)propan-1-one. It features a cyclopentanone ring connected via an amide bond to a benzene ring. The benzene ring has a chlorine atom at the 2-position and a long alkoxy chain at the 4-position.	 Chemical structure of 1-(2-chloro-4-nitrophenyl)-N,N'-bis(2-hydroxyethyl)benzidine. It consists of a benzidine core where one of the terminal phenyl rings is substituted with a chlorine atom at the 2-position and a nitro group at the 4-position. The other terminal ring is connected to a 2-hydroxyethyl chain.	EC number 428-240-5
2135874-53-0	 Chemical structure of 1-(2,4,6-triiodo-3-((2-hydroxy-1-(2-hydroxyethyl)amino)acetyl)oxyphenyl)propan-1-one. It features a central benzene ring with iodine atoms at the 2, 4, and 6 positions. At the 3-position, there is an ether linkage to a propanone chain, and at the 1-position, there is an amide linkage to a 2-hydroxyethyl chain.	 Chemical structure of 1-(2,4,6-triiodo-3-((2-hydroxy-1-(2-hydroxyethyl)amino)acetyl)oxyphenyl)propan-1-one. It features a central benzene ring with iodine atoms at the 2, 4, and 6 positions. At the 3-position, there is an ether linkage to a propanone chain, and at the 1-position, there is an amide linkage to a 2-hydroxyethyl chain.	EC number 430-120-2

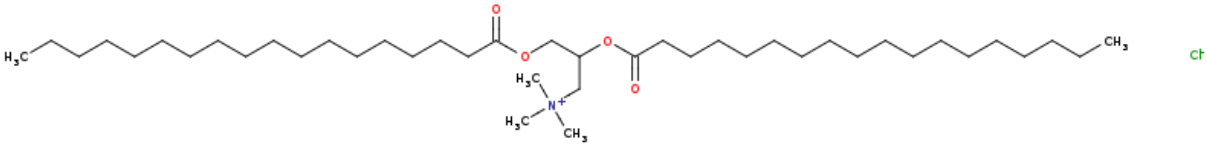
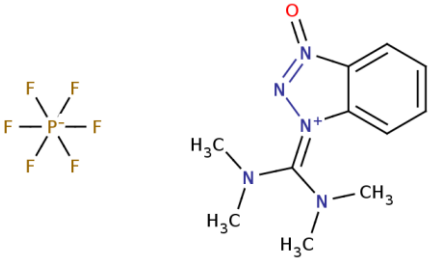
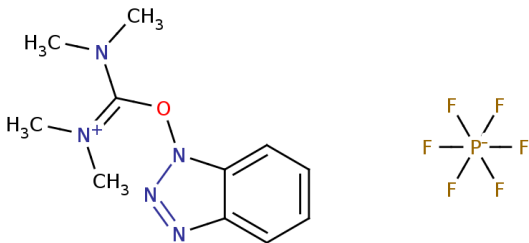
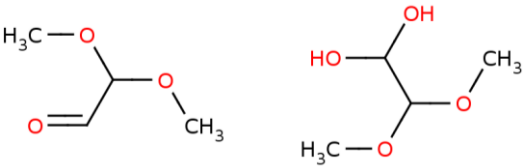
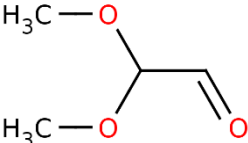
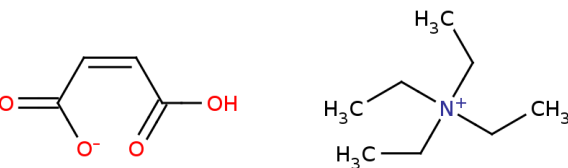
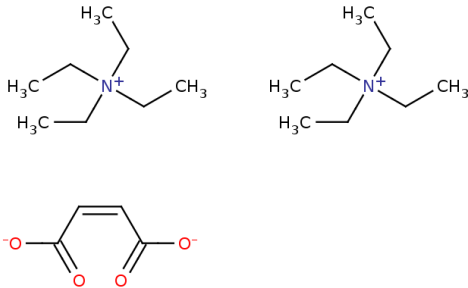
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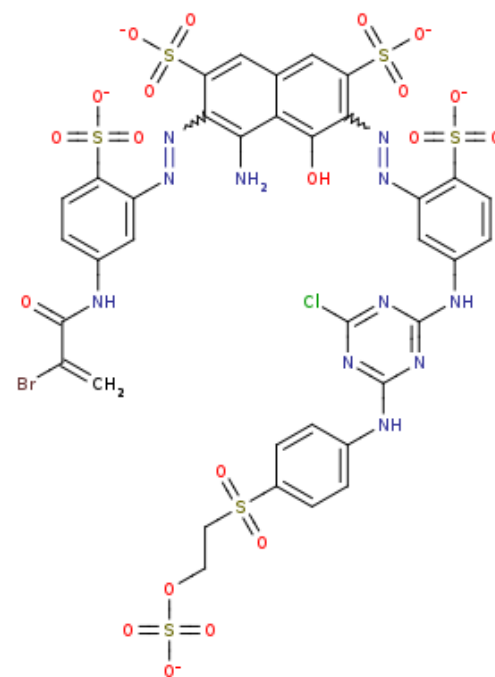
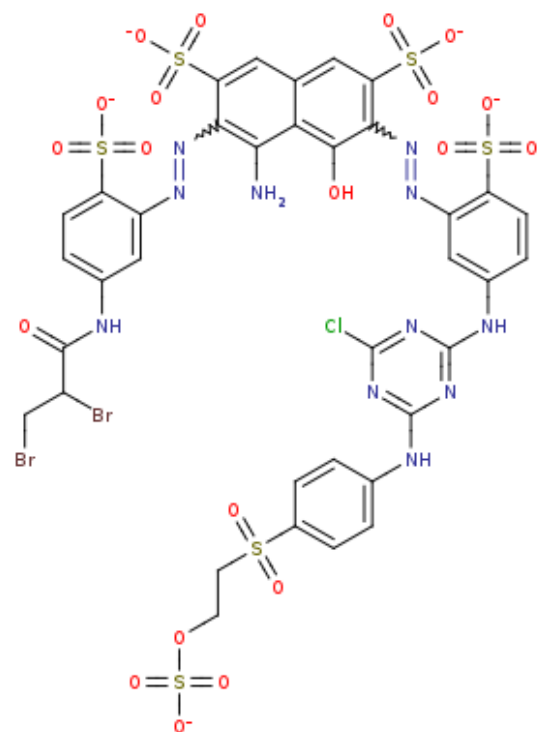
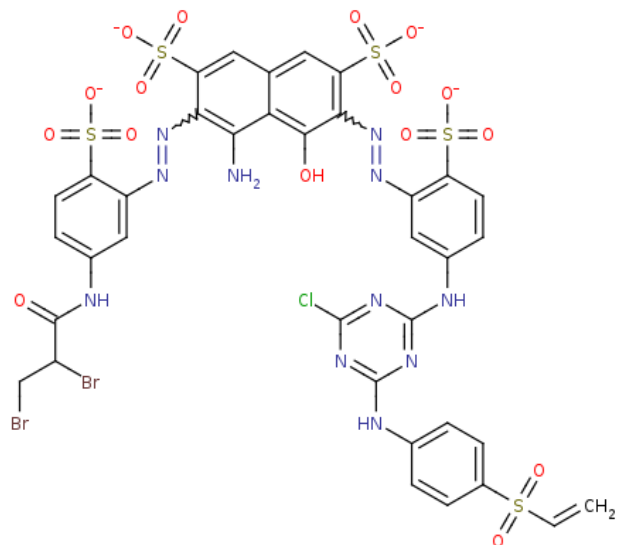
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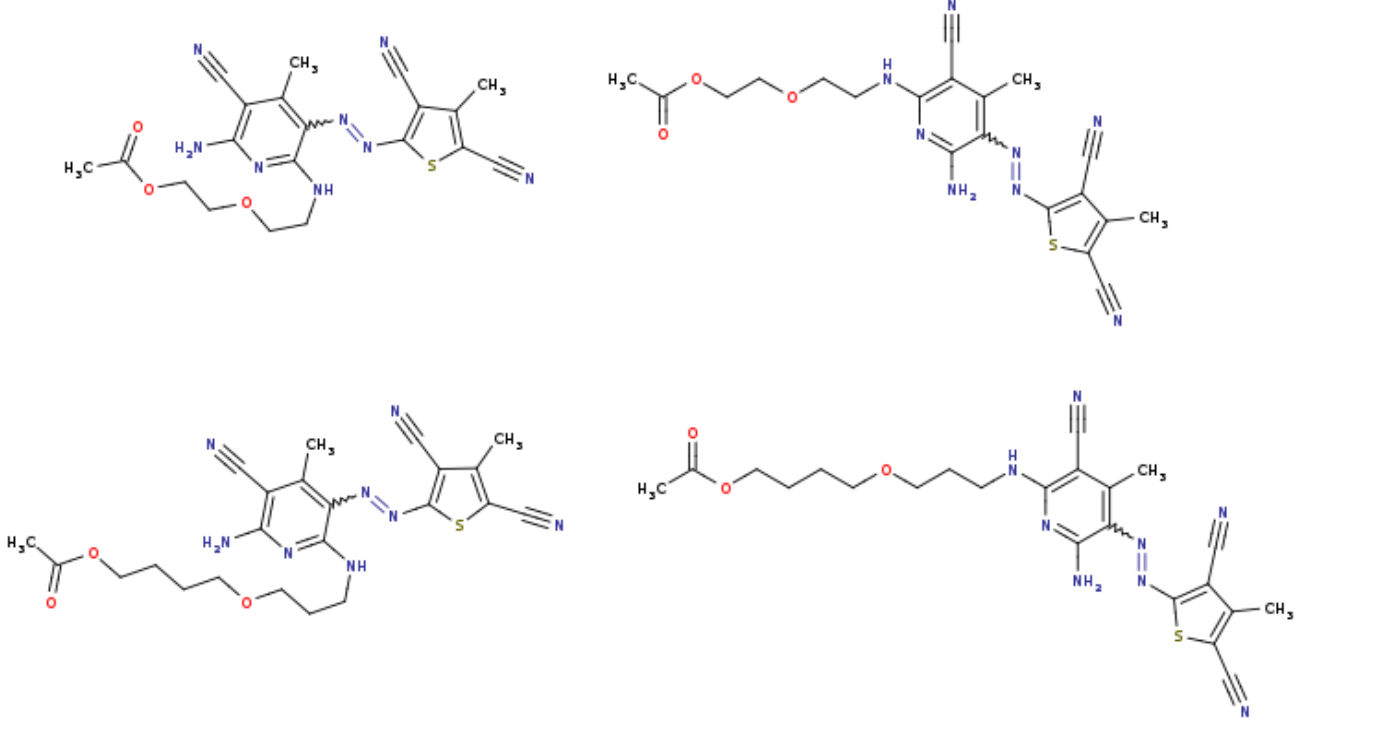
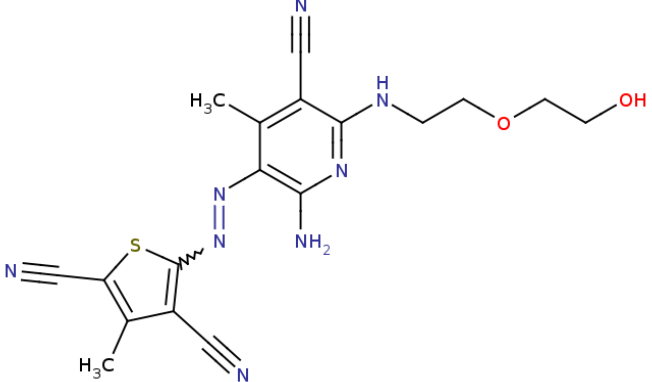
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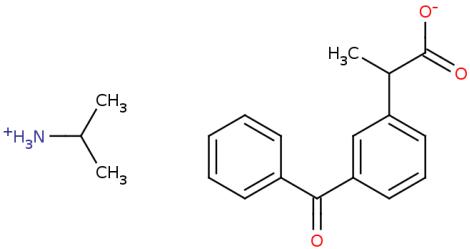
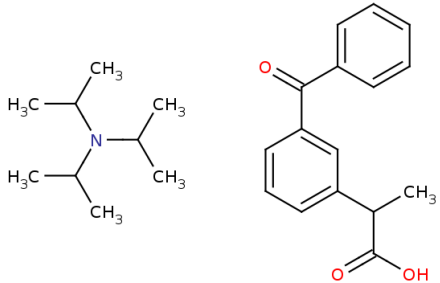
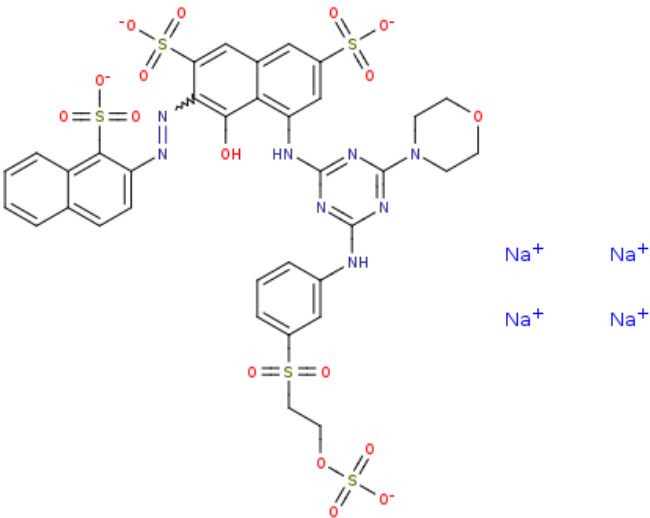
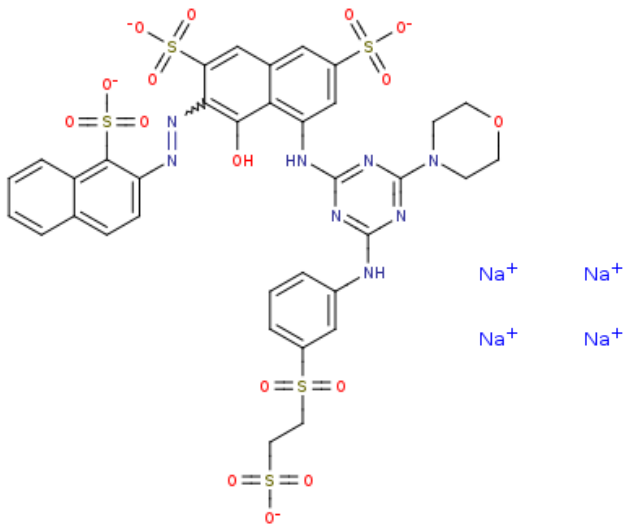
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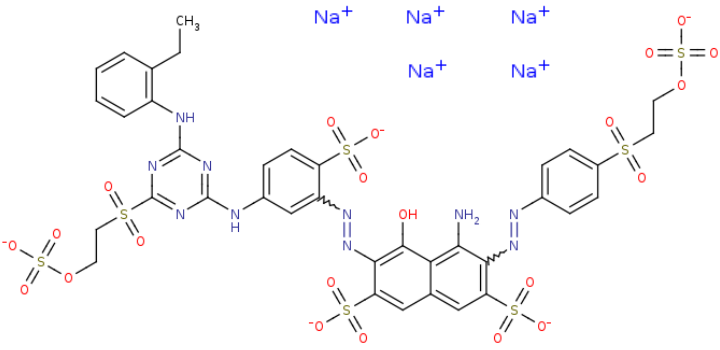
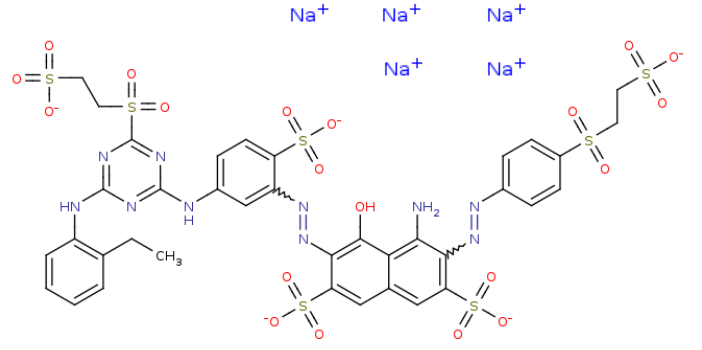
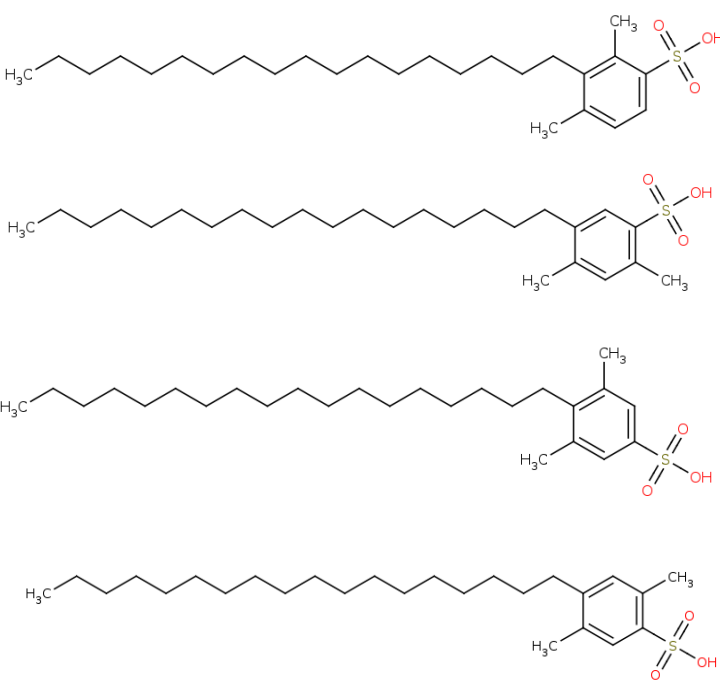
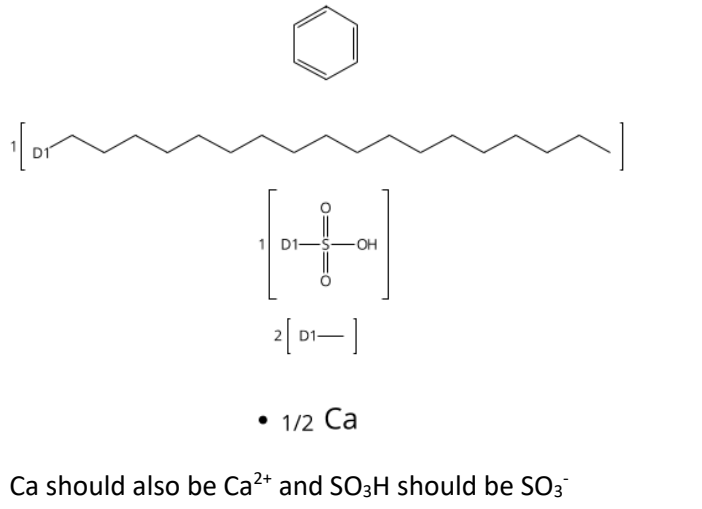


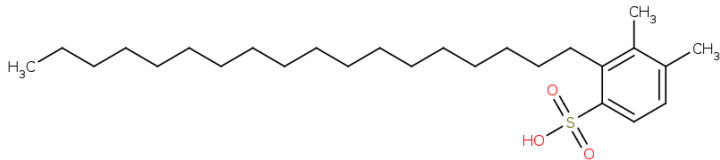
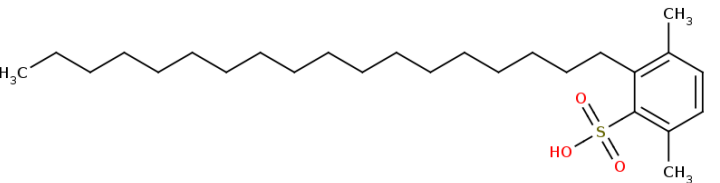
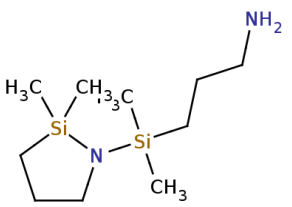
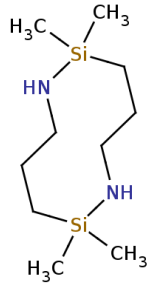
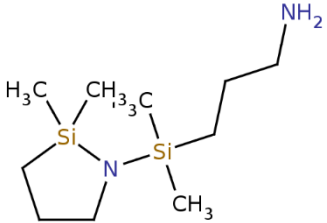
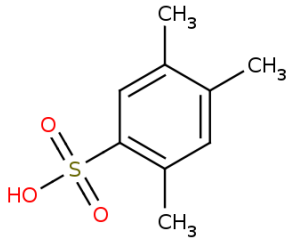
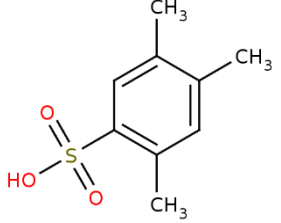
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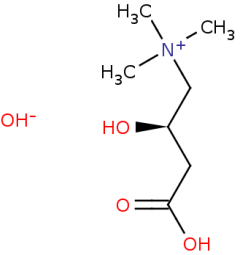
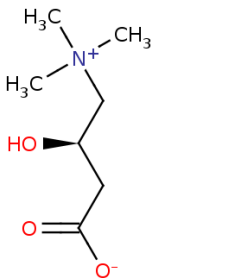
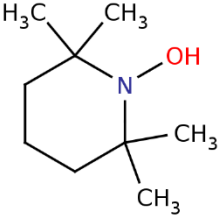
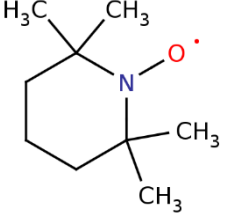
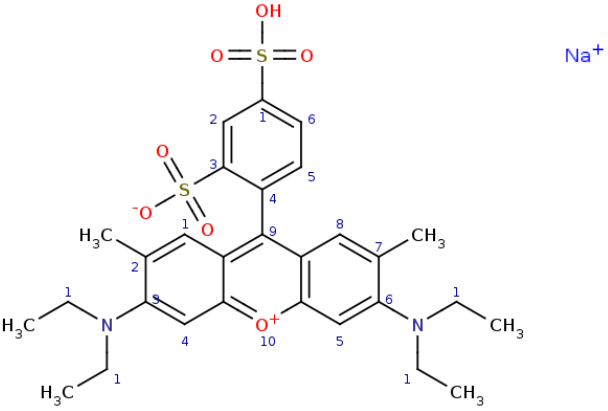
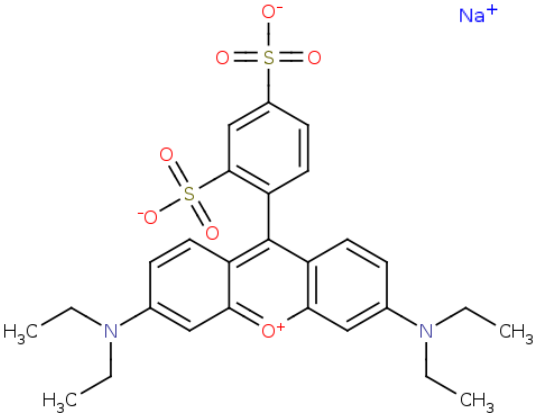
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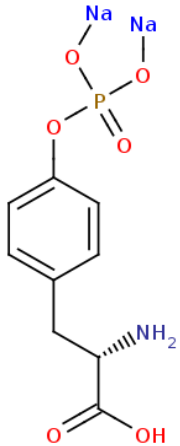
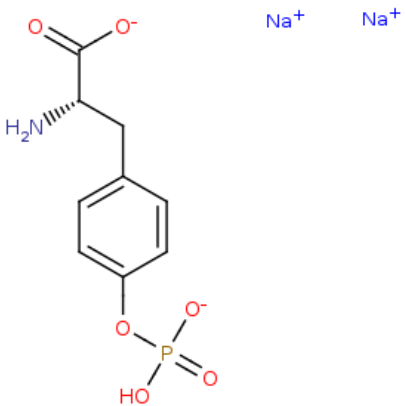
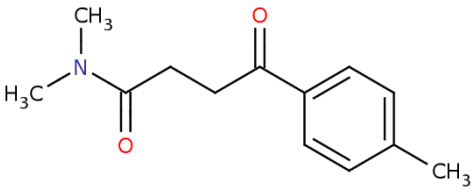
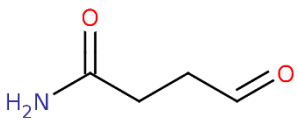
107815-88-3 (incorrect form)		EC number 410-530-8
107815-88-3 (correct form)		EC number 410-530-8

1379932-74-7	 Chemical structure of 2-(dimethylamino)acetic acid (DMAA) and 2-phenyl-2-phenylpropanoic acid (PPA).	 Chemical structure of 2-(dimethylamino)acetic acid (DMAA) and 2-phenyl-2-phenylpropanoic acid (PPA).	EC number 417-970-1
1379676-82-0	 Chemical structure of a complex sulfonamide derivative, featuring a naphthalene ring system, a pyrimidine ring, and a morpholine ring. The structure includes four sodium counterions (Na⁺).	 Chemical structure of a complex sulfonamide derivative, featuring a naphthalene ring system, a pyrimidine ring, and a morpholine ring. The structure includes four sodium counterions (Na⁺).	EC number 413-070-6

1379676-74-0			EC number 423-790-2
148262-93-5		 Ca should also be Ca^{2+} and SO_3H should be SO_3^-	EC number 402-040-8

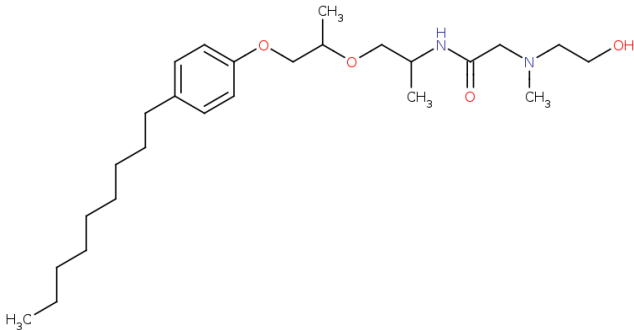
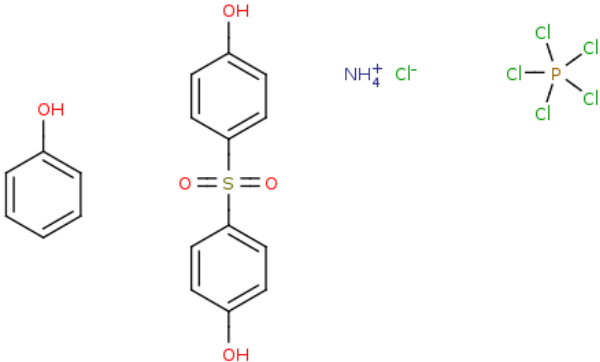
	  CaH_2 (v2) 6x		
388606-32-4	 		EC number 470-090-8
3453-84-7	 H_2O H_2O		EC number 420-770-5

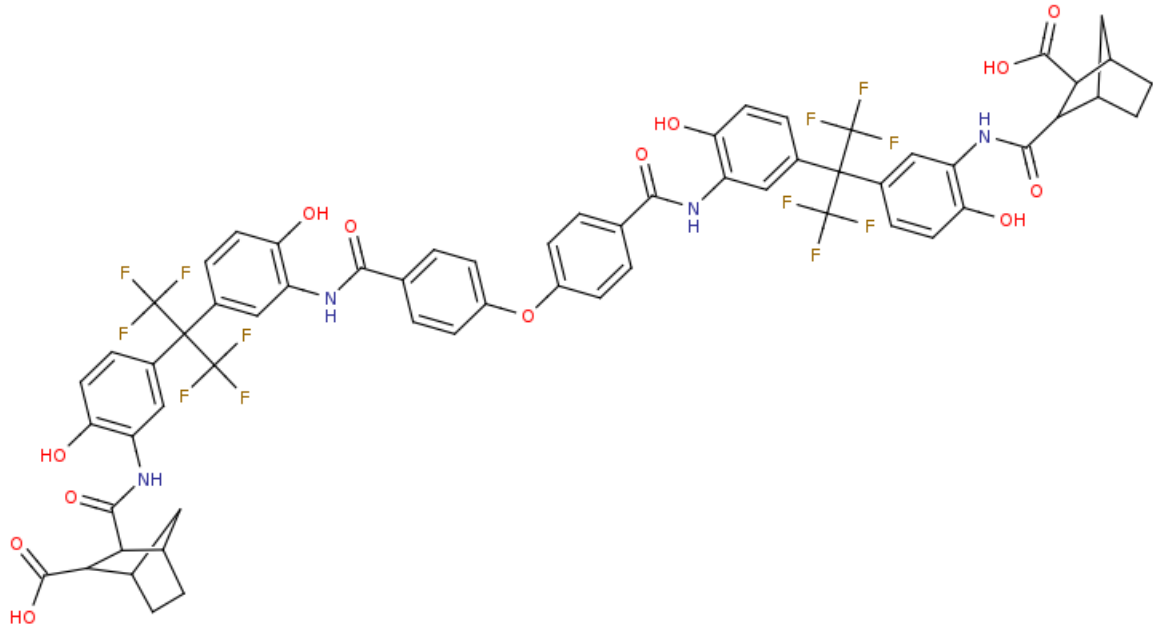
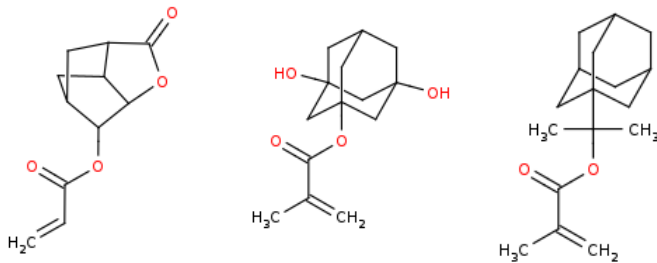
541-15-1			EC number 208-768-0
2564-83-2			EC number 219-888-8
3520-42-1			EC number 222-529-8

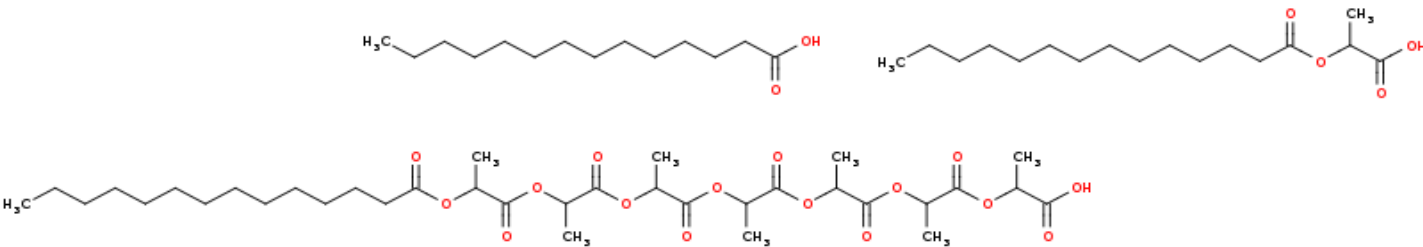
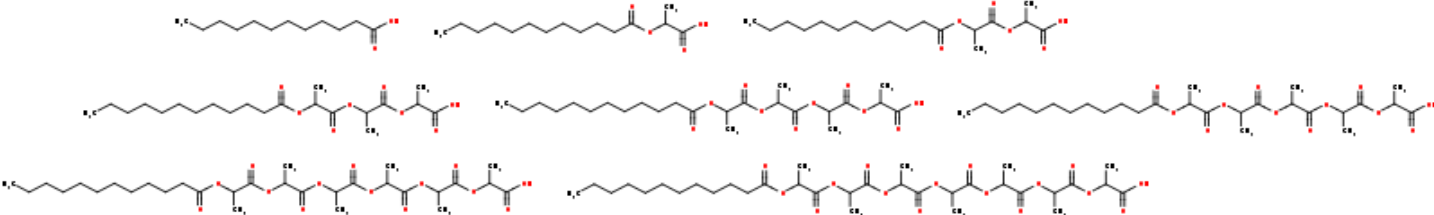
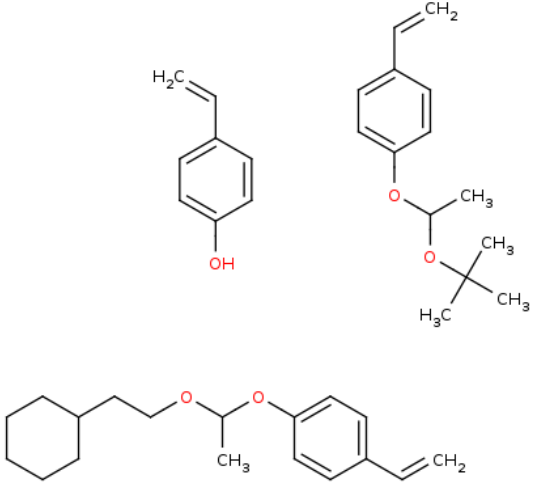
1610350-91-8			EC number 860-352-3
27719-81-9			EC number 464-950-1

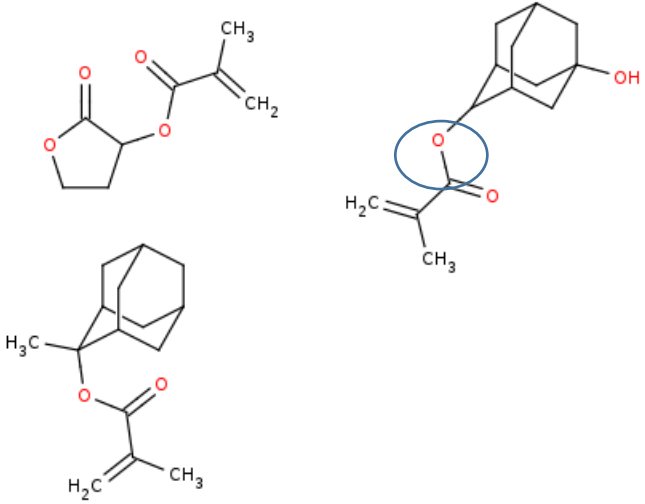
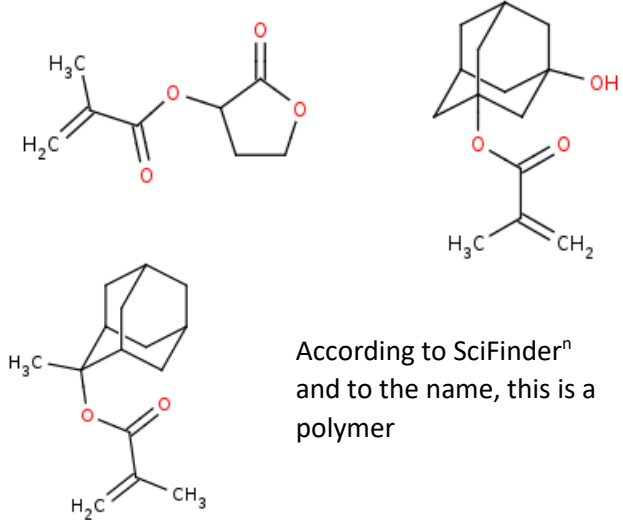
2) Monomer shown for a polymer

Table 2: Structures in the ECHA database for organic mono-constituent substances as of January 2022 that show most probably monomers although the name or CAS RN™ says polymer.

CAS RN™	Structure in the database	Structure corresponding to the CAS RN™	Comment
144736-29-8		According to SciFinder ⁿ and to the name, this is a polymer.	EC number 413-420-8
260408-02-4		According to SciFinder ⁿ and to the name, this is a polymer.	EC number 439-270-3

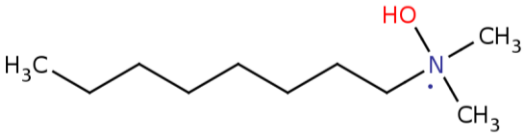
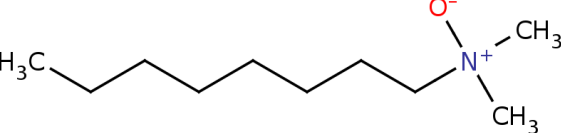
-		EC number 426-580-9	
	According to the name, this is a polymer (POLYAMIDE RESIN)		
-		According to the name, this is a polymer (2-Propenoic acid, 2-methyl-, 3,5-dihydroxytricyclo[3.3.1.1 ^{3,7}]dec-1-yl ester, polymer with hexahydro-2-oxo-3,5-methano-2H-cyclopenta[b]furan-6-yl 2-propenoate and 1-methyl-1-tricyclo[3.3.1.1 ^{3,7}]dec-1-ylethyl-2-methyl-2-propenoate)	EC number 473-380-2

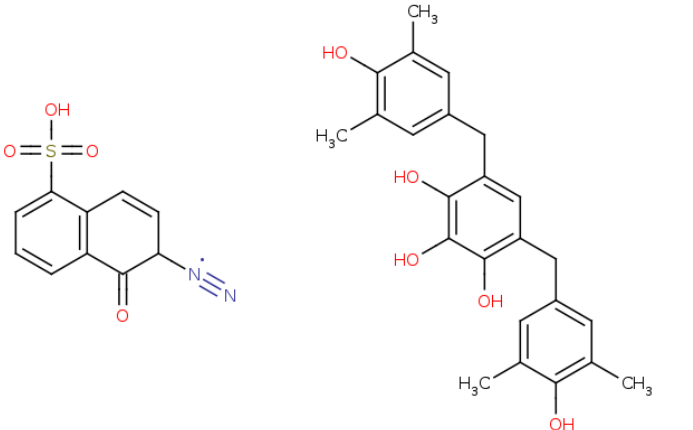
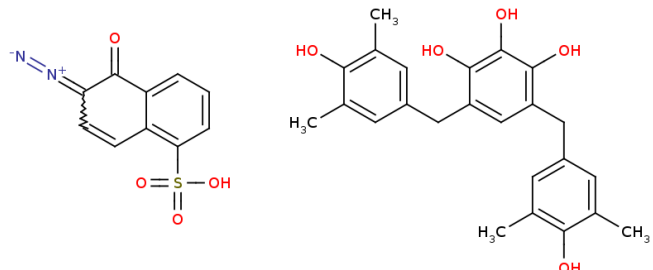
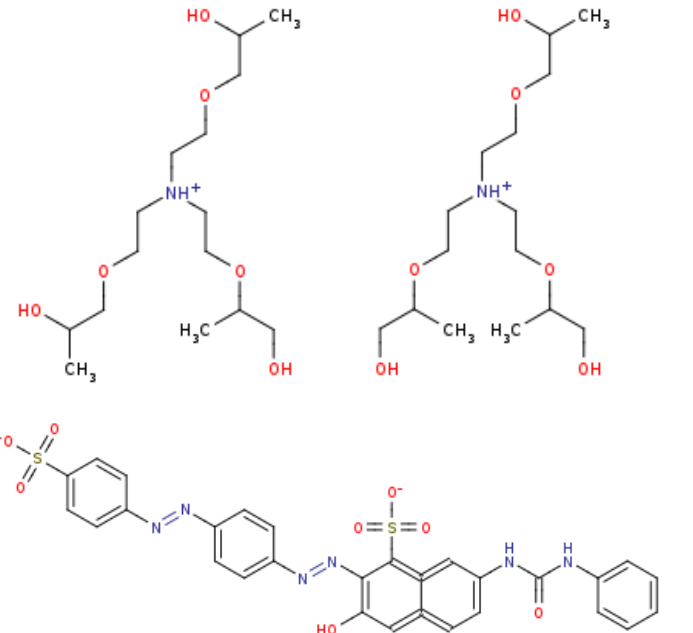
174591-51-6	 According to SciFinderⁿ and to the name, this is a polymer.	EC number 412-580-6
58856-63-6	 According to SciFinderⁿ and to the name, this is a polymer.	EC number 412-590-0
-		According to the name, this is a polymer (Phenol, 4-ethenyl-, homopolymer, 1-(2-cyclohexylethoxy)ethyl ethers) EC number 484-300-0

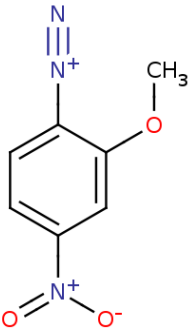
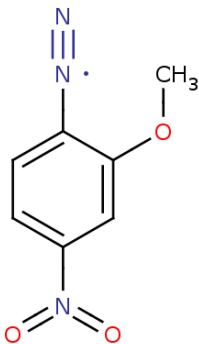
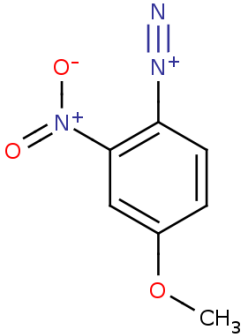
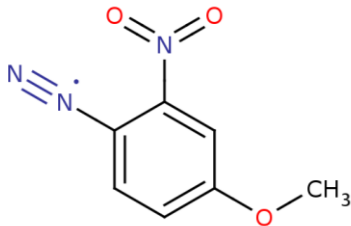
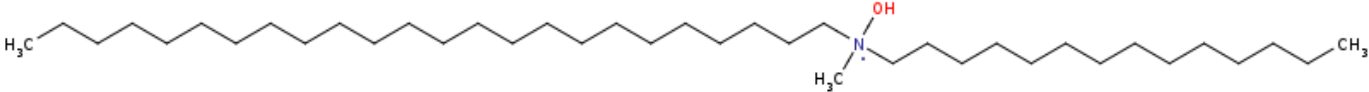
258879-87-7		 According to SciFinderⁿ and to the name, this is a polymer	EC number 442-950-2
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3) Unusual valence

Table 3: Structures with unusual valence in the ECHA database for organic mono-constituent substances as of January 2022.

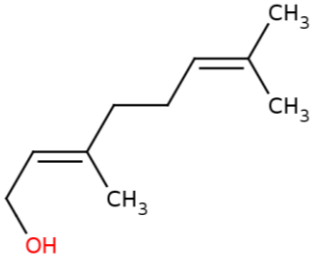
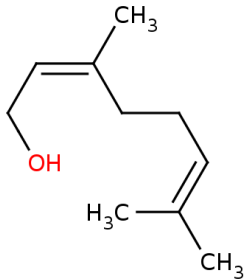
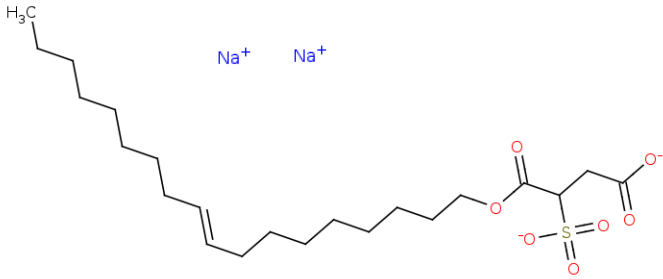
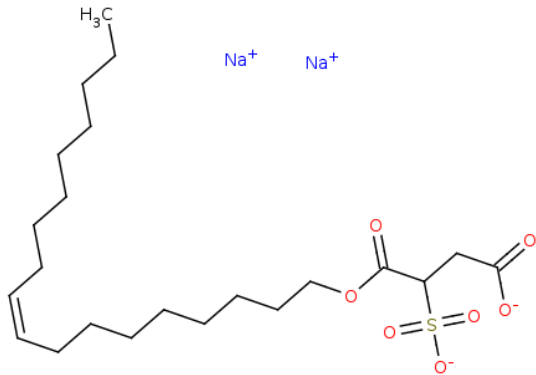
CAS RN™	Structure in the database	Structure corresponding to the CAS RN™	Comment
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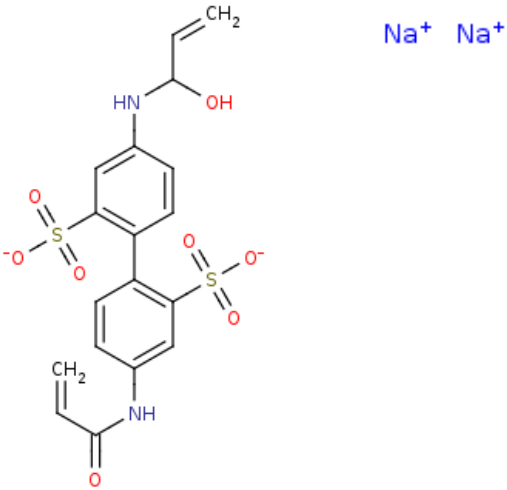
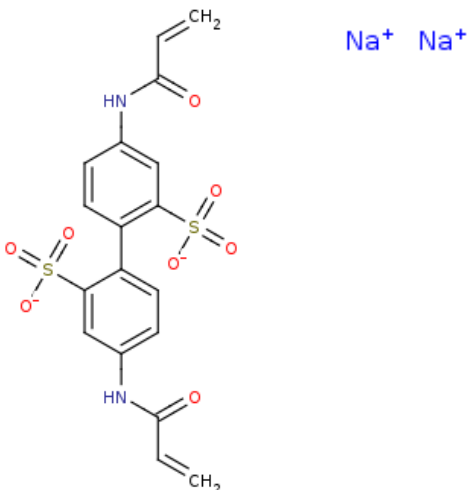
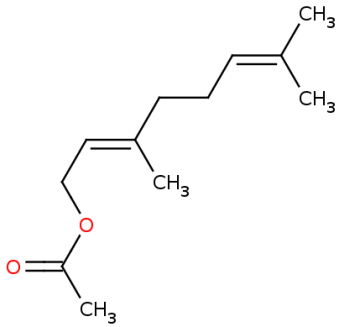
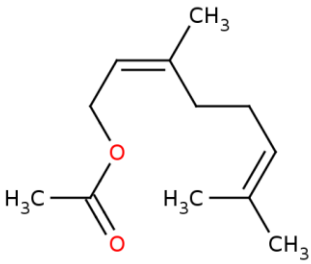
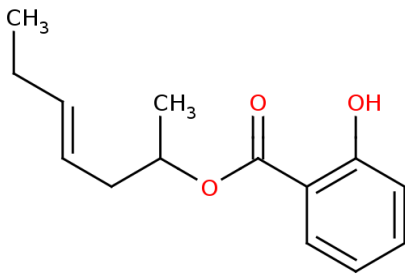
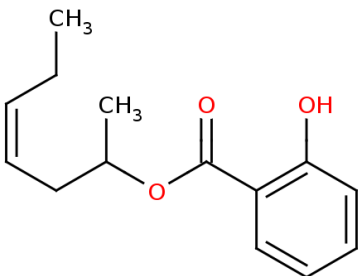
133686-87-0			EC number 451-140-8
1628433-99-7		Carbon should only have 4 bonds and not 5. Correct strucutre is not available elsewhere	EC number 406-170-6

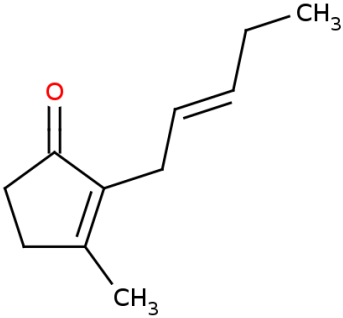
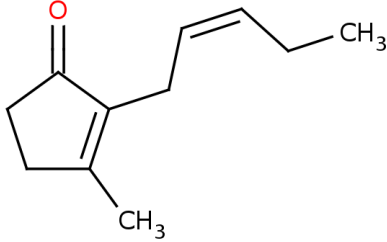
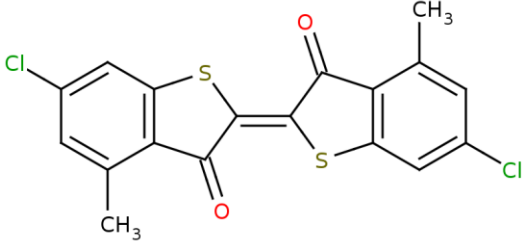
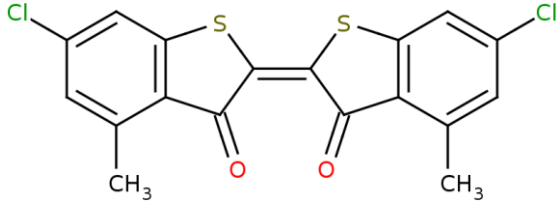
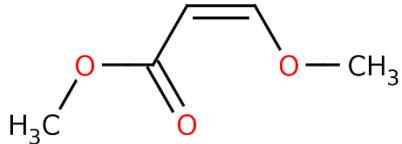
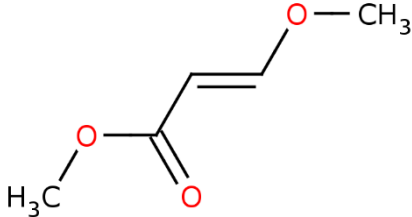
27761-26-8			EC number 248-642-2
27165-25-9			EC number 248-284-7
- (incorrect form)			EC number 440-250-1
- (correct form)	Substance could not be identified in any of the other databases		EC number 440-250-1

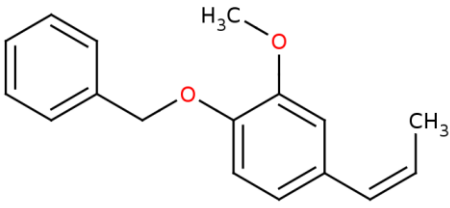
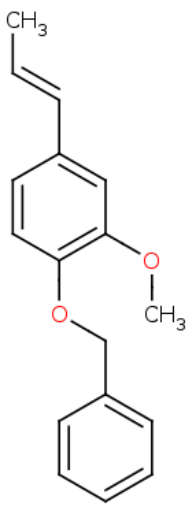
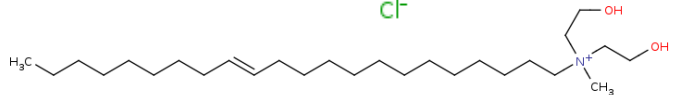
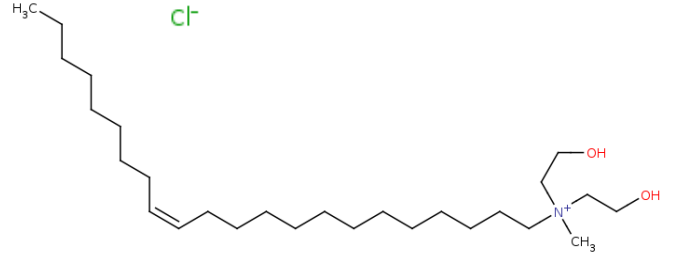
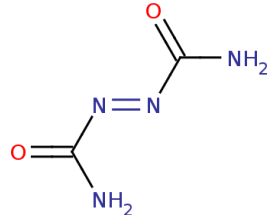
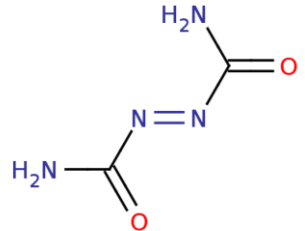
4) Inconsistency related to cis/trans isomers

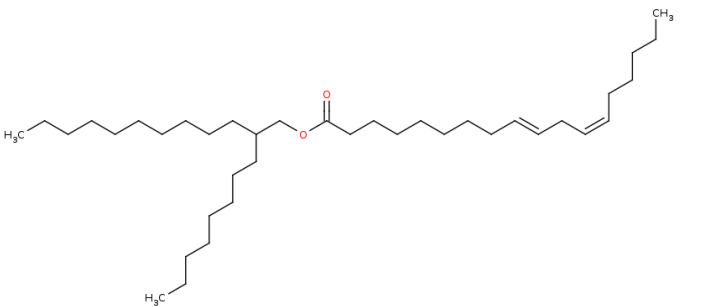
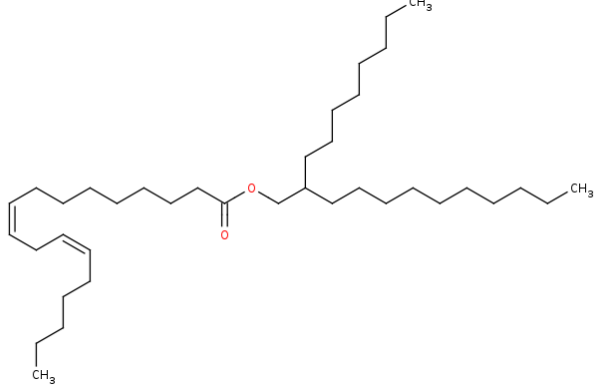
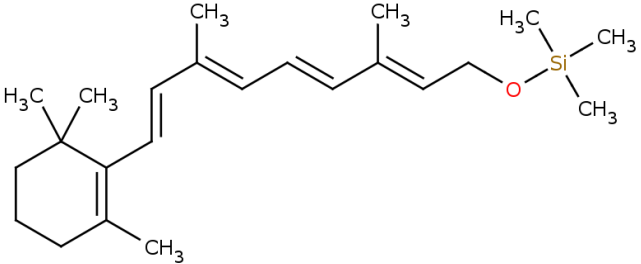
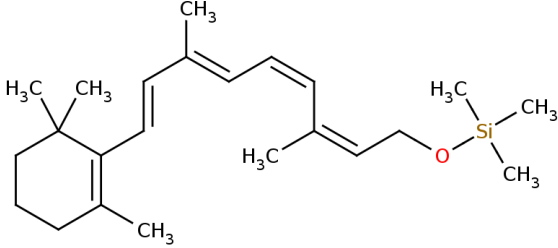
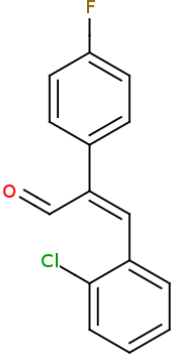
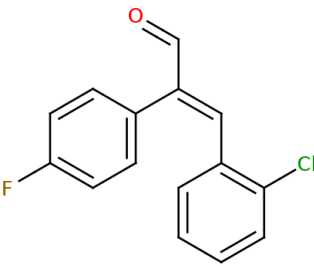
Table 4: Substances in the ECHA database where the SMILES do not correspond to the CAS RN™ as allocated in SciFinderⁿ. The reason for the mismatches here are deviations in the cis/trans isomers.

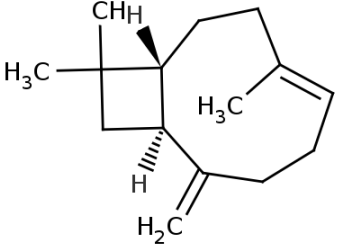
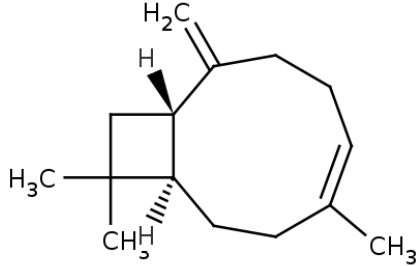
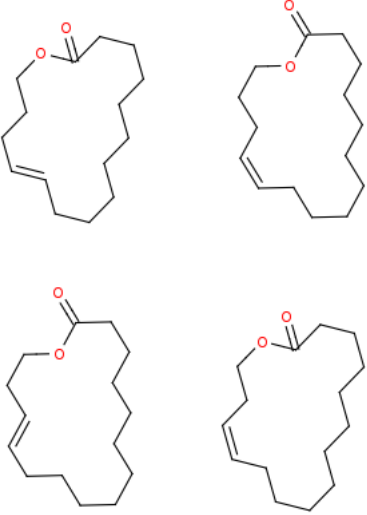
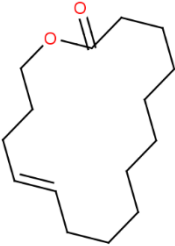
CAS RN™	Structure in the database	Structure corresponding to the CAS RN™	Comment
106-25-2			EC number 203-378-7
94213-67-9			EC number 303-773-5

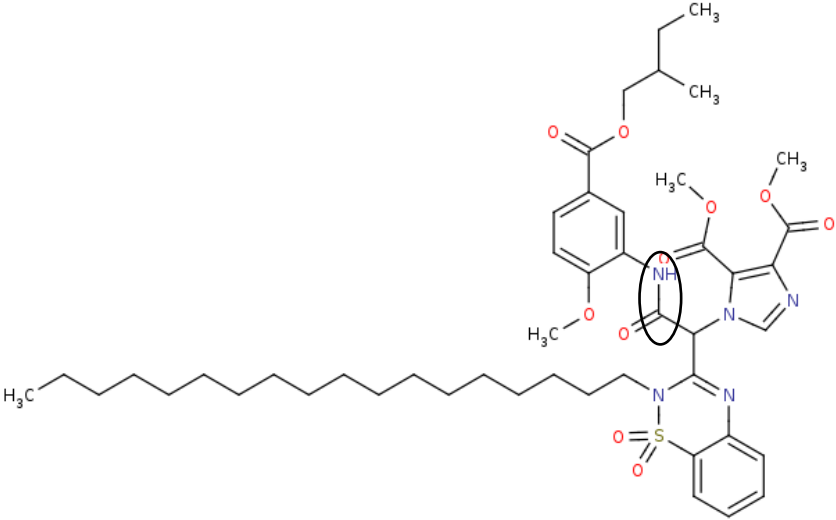
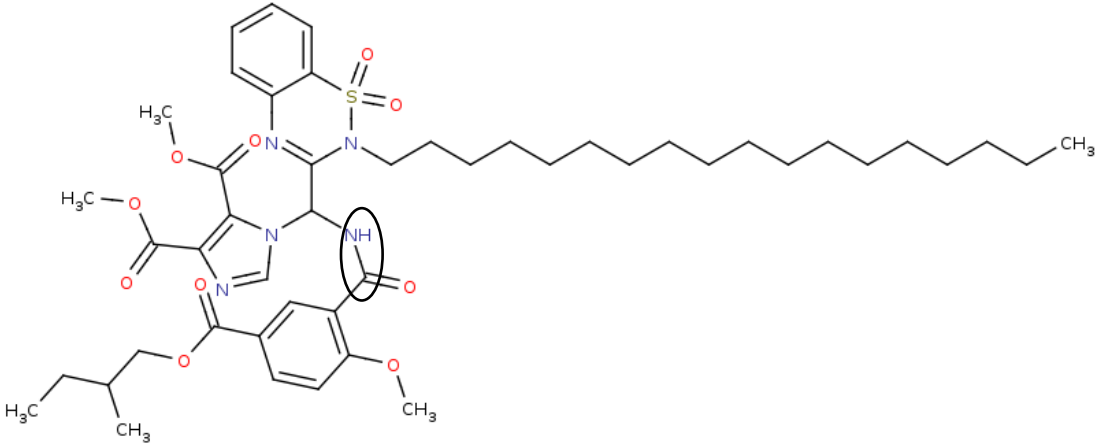
881539-89-5			EC number 812-549-0
141-12-8			EC number 205-459-2
873888-84-7			EC number 700-488-1

488-10-8	 <chem>CCCC=Cc1c(C)c(c(c1)O=)C=C</chem>	 <chem>CCCC=Cc1c(C)c(c(c1)O=)C=C</chem>	EC number 207-668-4
2379-74-0	 <chem>Cc1cc(Cl)cc2sc(cc12)C(=O)C3=C(C(=O)S4C=C(Cl)C=C4C)S5C6=CC=C(Cl)C=C6C(=O)S53</chem>	 <chem>Cc1cc(Cl)cc2sc(cc12)C(=O)C3=C(C(=O)S4C=C(Cl)C=C4C)S5C6=CC=C(Cl)C=C6C(=O)S53</chem>	EC number 219-163-6
5788-17-0	 <chem>COC(=O)C(=O)/C=C/C(=O)OC</chem>	 <chem>COC(=O)C(=O)/C=C/C(=O)OC</chem>	EC number 412-900-4

120-11-6	 <chem>COc1cc(C=C)cc(OCc2ccccc2)c1</chem>	 <chem>COc1cc(C=C)cc(OCc2ccccc2)c1OC</chem>	EC number 204-370-6
120086-58-0	 <chem>CCCCCCCCC/C=C\CCCCCCCCCCCCCCCC[N+](C)(C)CCO.[Cl-]</chem>	 <chem>CCCCCCCCC/C=C\CCCCCCCCCCCCCCCC[N+](C)(C)CCO.[Cl-]</chem>	EC number 426-210-6
123-77-3	 <chem>NC(=O)NNC(=O)N</chem>  <chem>NC(=O)NNC(=O)N</chem>	 <chem>NC(=O)NNC(=O)N</chem>	EC number 204-650-8 CAS RN™ does not cover both forms

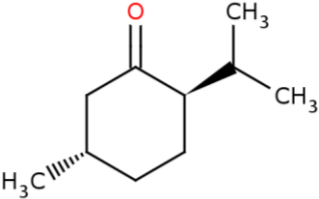
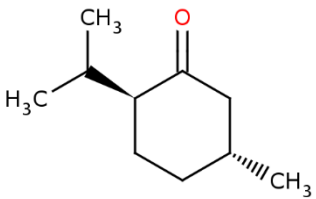
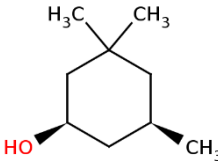
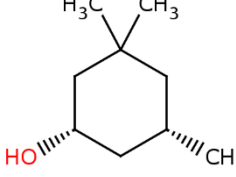
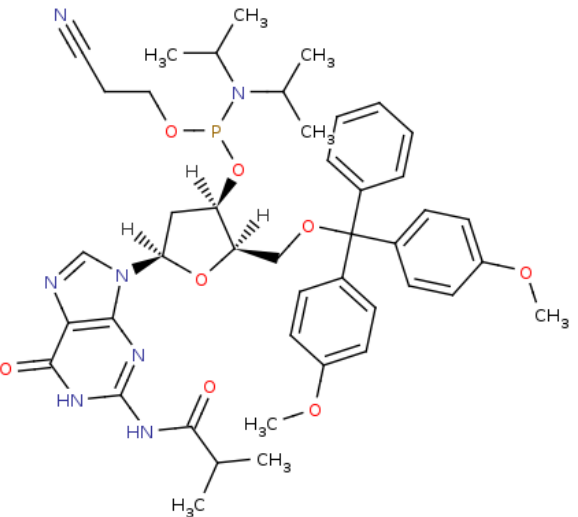
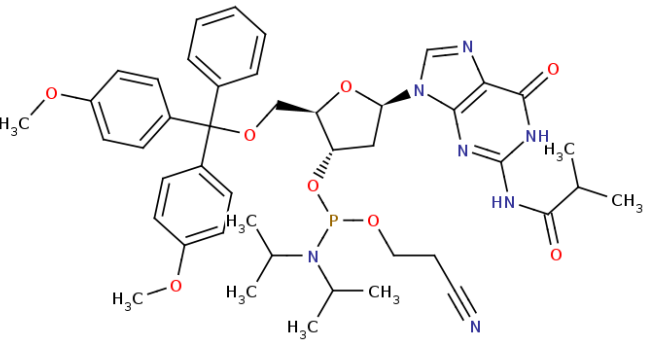
129423-60-5	 Chemical structure of a branched ester. The left side is a branched alkyl chain with a methyl group at the end of one branch and a methyl group at the end of the main chain. The right side is a long chain containing two double bonds and a terminal methyl group.	 Chemical structure of a branched ester. The left side is a long chain containing two double bonds and a terminal methyl group. The right side is a branched alkyl chain with a methyl group at the end of one branch and a methyl group at the end of the main chain.	EC number 438-100-5
16729-19-4	 Chemical structure of a complex molecule. It features a cyclohexene ring with two methyl groups on one carbon and a methyl group on another. Attached to the ring is a long chain with three double bonds and a trimethylsilyl group at the end.	 Chemical structure of a complex molecule. It features a cyclohexene ring with two methyl groups on one carbon and a methyl group on another. Attached to the ring is a long chain with three double bonds and a trimethylsilyl group at the end.	EC number 435-930-1
112704-51-5	 Chemical structure of a molecule. It consists of a benzene ring with a chlorine atom at the 2-position and a side chain at the 1-position. The side chain includes a double bond and a fluorine atom.	 Chemical structure of a molecule. It consists of a benzene ring with a chlorine atom at the 2-position and a side chain at the 1-position. The side chain includes a double bond and a fluorine atom.	EC number 410-980-5

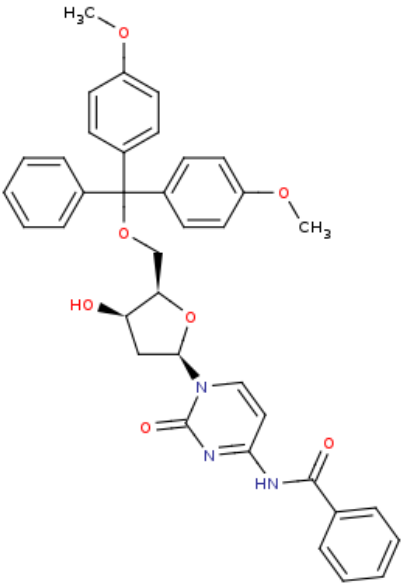
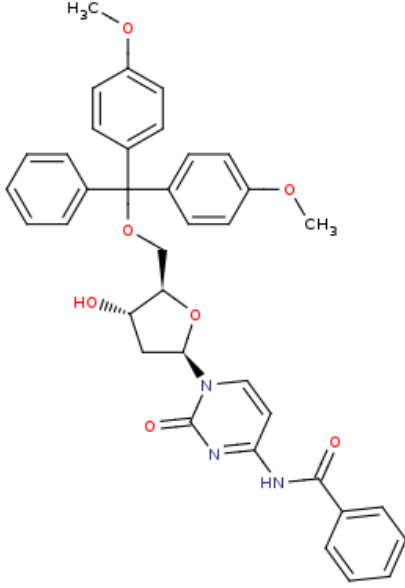
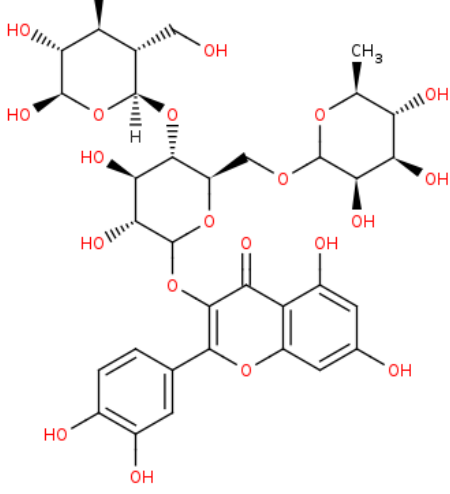
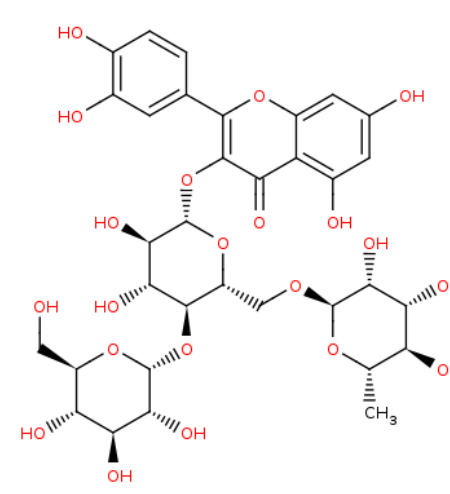
87-44-5			EC number 201-746-1
111879-80-2			EC number 422-320-3

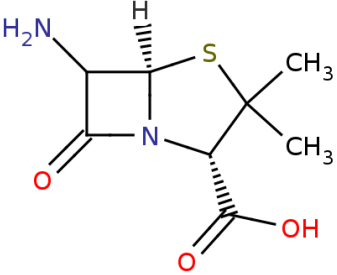
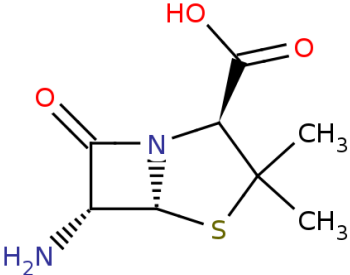
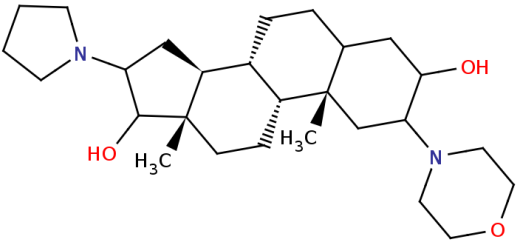
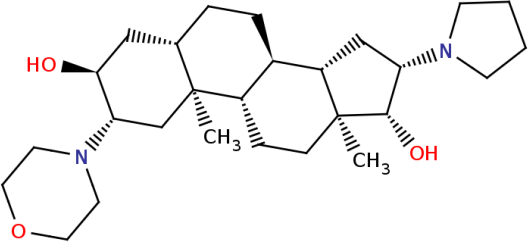
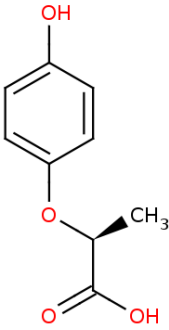
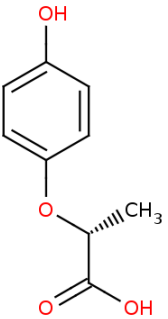
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1380163-91-6 (correct form)		EC number 443-910-7

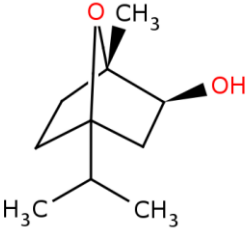
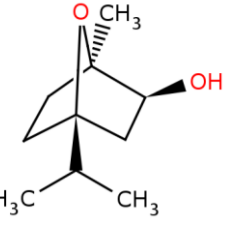
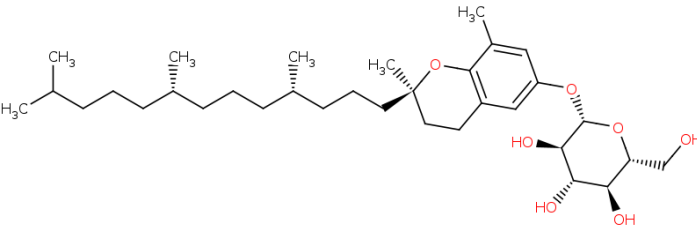
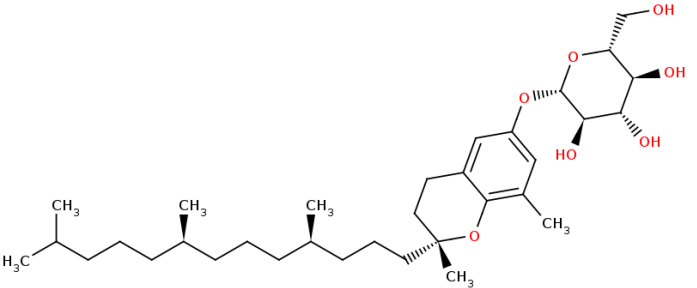
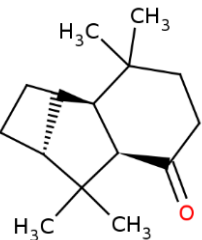
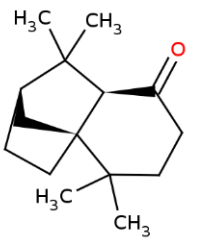
5) Inconsistencies related to the stereochemistry (deviating stereochemistry)

Table 5: Substances in the ECHA database where the SMILES do not correspond to the CAS RN™ as allocated in SciFindern. The reason for the mismatches here are deviations in the stereochemistry.

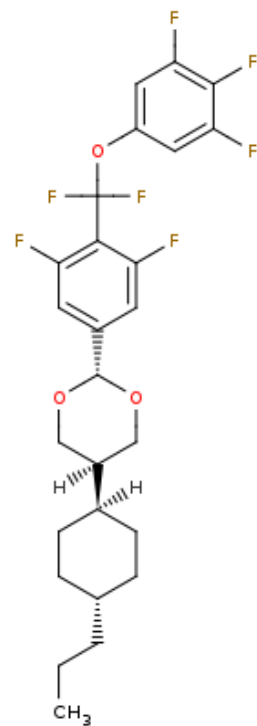
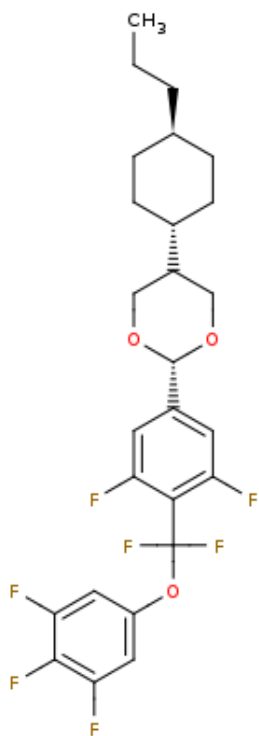
CAS RN™	Structure in the database	Structure corresponding to the CAS RN™	Comment
89-80-5			EC number 201-941-1
933-48-2			EC number 213-268-0
93183-15-4			EC number 685-519-6

67219-55-0			EC number 266-605-9
130603-71-3			EC number 424-170-4

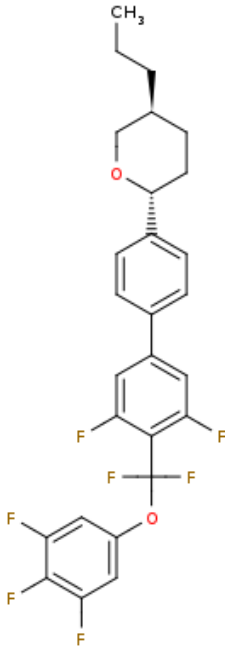
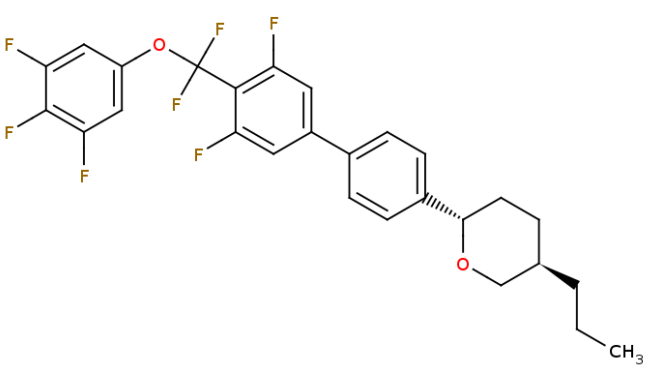
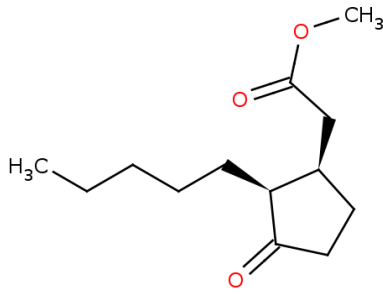
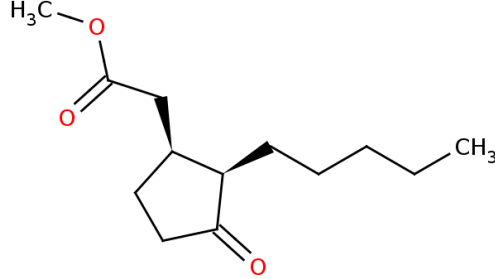
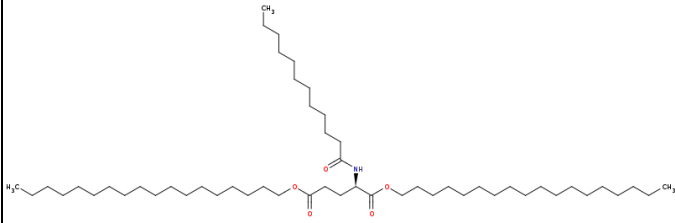
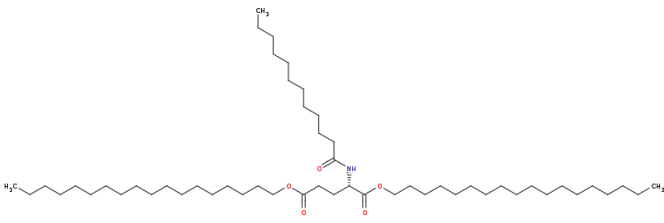
551-16-6			EC number 208-993-4
119302-20-4			EC number 601-595-5
94050-90-5			EC number 407-960-3

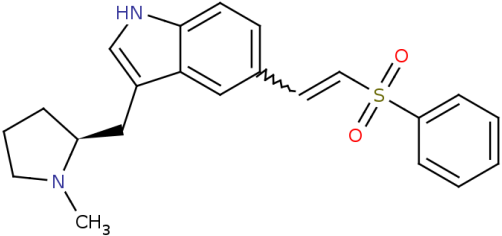
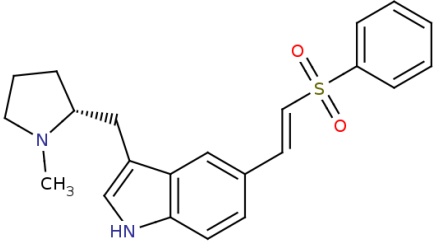
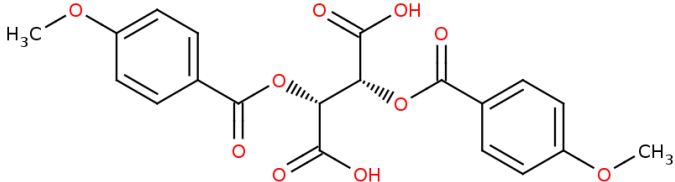
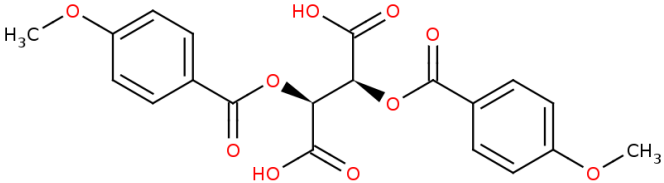
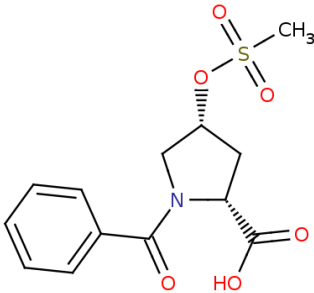
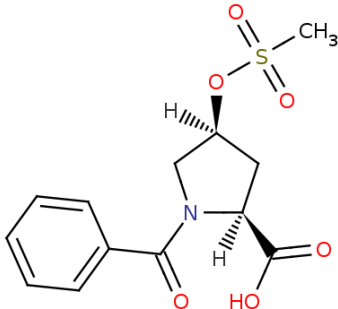
87172-89-2	 Chemical structure of 1-methoxy-2-methyl-4-hydroxy-4,5,6,7-tetrahydronaphthalene. It features a bicyclic system with a methoxy group (OCH₃) at position 1, a methyl group (CH₃) at position 2, and a hydroxyl group (OH) at position 4.	 Chemical structure of 1-methoxy-2-methyl-4-hydroxy-4,5,6,7-tetrahydronaphthalene. It features a bicyclic system with a methoxy group (OCH₃) at position 1, a methyl group (CH₃) at position 2, and a hydroxyl group (OH) at position 4.	EC number 402-470-6
102340-61-4	 Chemical structure of a complex glycoside. It consists of a long alkyl chain with several methyl branches, connected via an ether linkage to a benzene ring. The benzene ring is further connected to a sugar moiety (a pyranose ring) which has multiple hydroxyl groups (OH) and a methoxy group (OCH₃).	 Chemical structure of a complex glycoside. It consists of a long alkyl chain with several methyl branches, connected via an ether linkage to a benzene ring. The benzene ring is further connected to a sugar moiety (a pyranose ring) which has multiple hydroxyl groups (OH) and a methoxy group (OCH₃).	EC number 805-675-2
29461-13-0	 Chemical structure of a bicyclic ketone. It features a bicyclic system with a ketone group (C=O) and several methyl groups (CH₃).	 Chemical structure of a bicyclic ketone. It features a bicyclic system with a ketone group (C=O) and several methyl groups (CH₃).	EC number 249-648-8

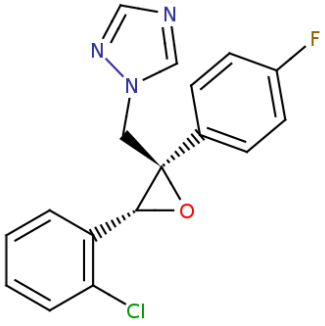
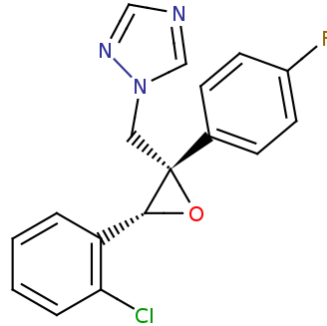
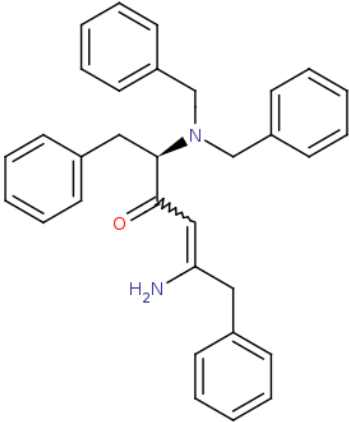
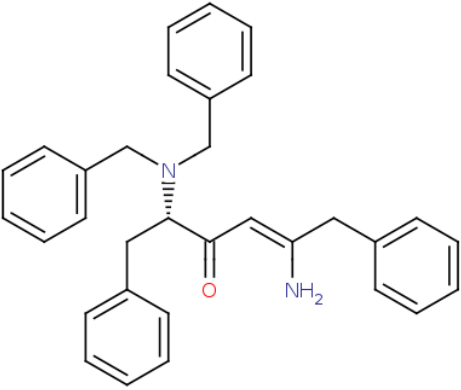
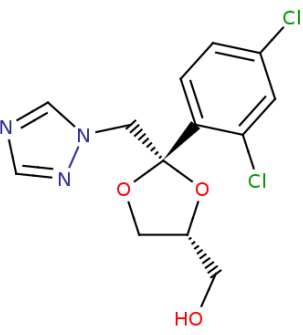
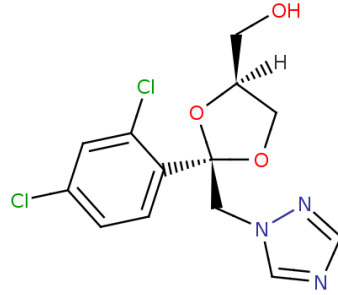
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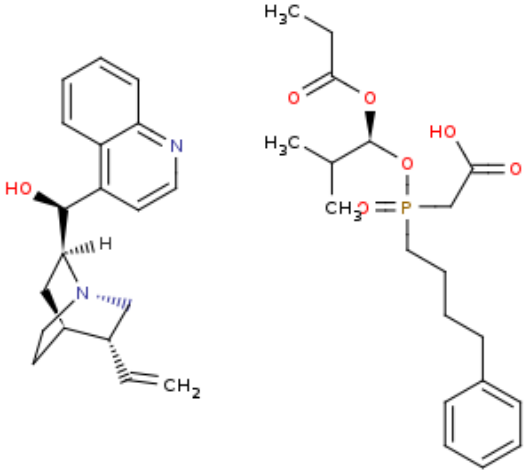
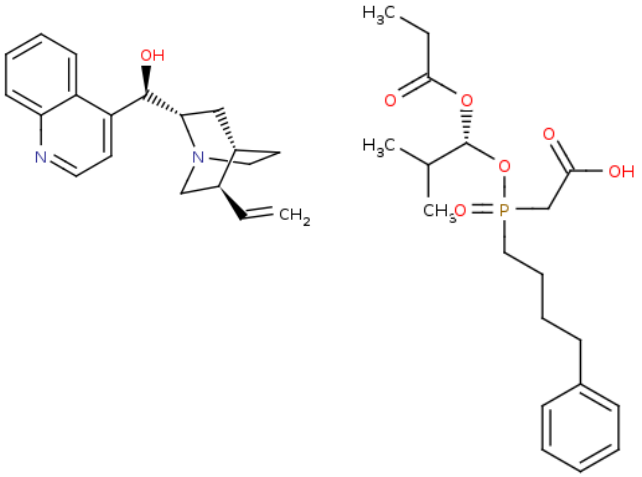
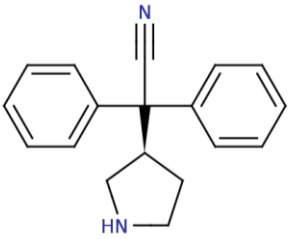
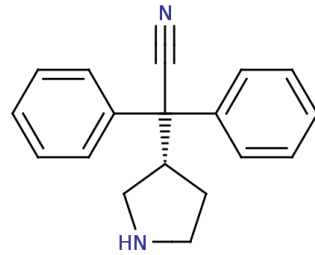


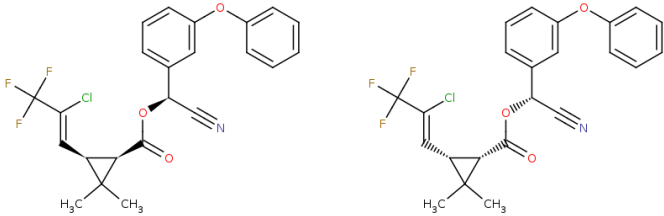
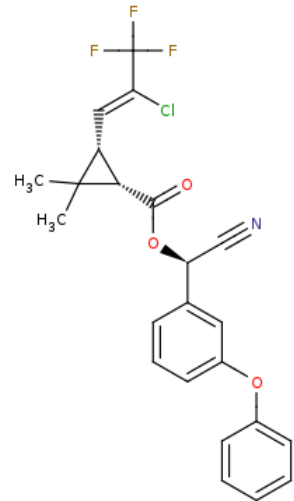
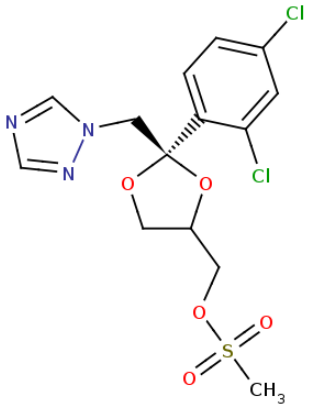
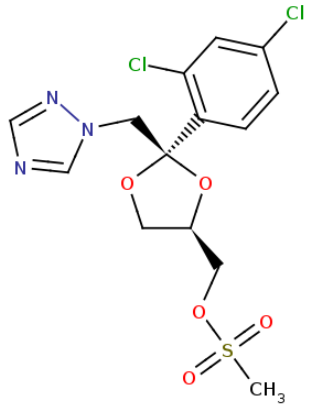
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700-701-8

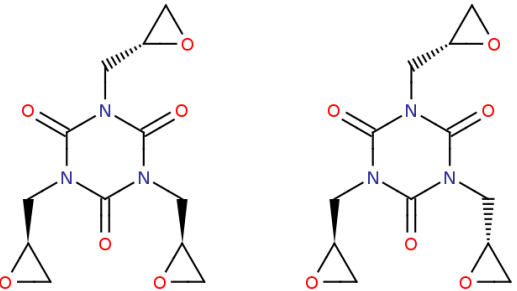
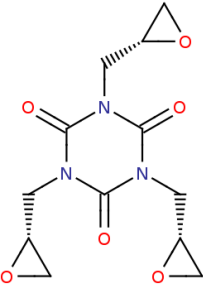
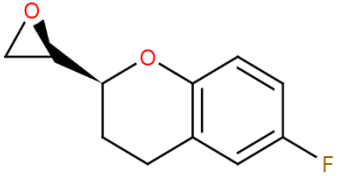
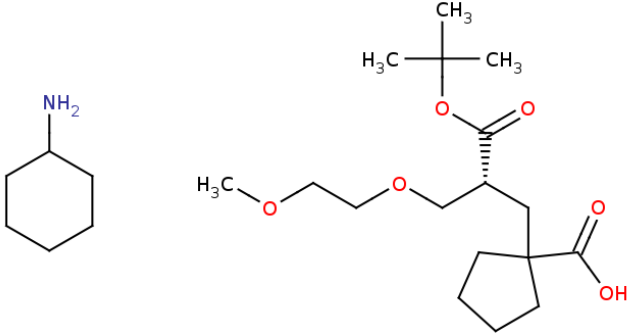
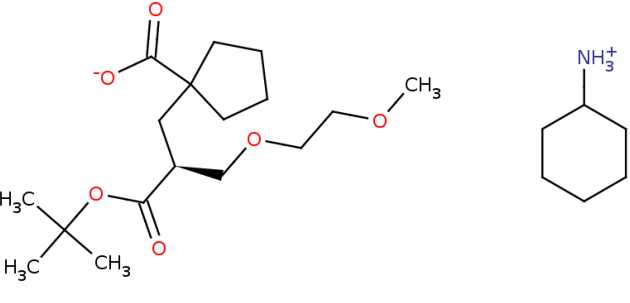
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55258-21-4			EC number 807-033-7

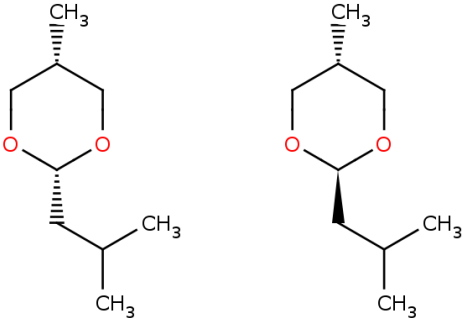
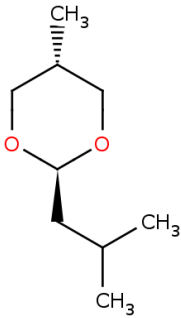
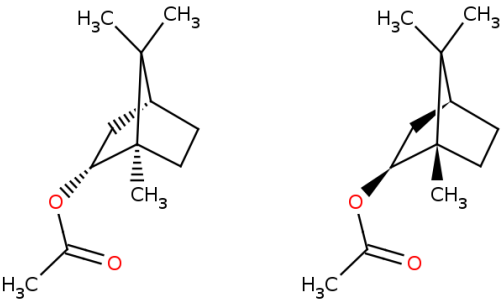
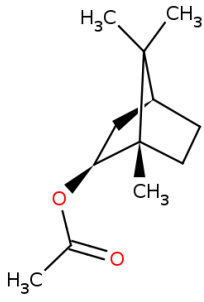
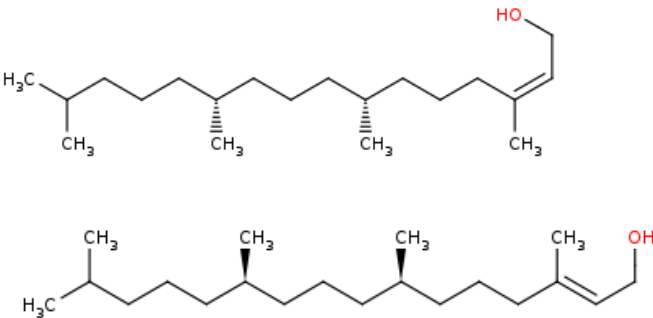
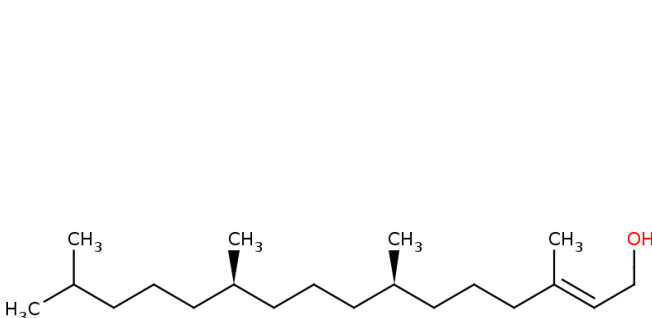
180637-89-2	 Chemical structure of 1-methyl-2-((E)-3-phenylsulfonyl-2-propenyl)-1H-indole-3-ylpyrrolidine. It features a pyrrolidine ring with a methyl group on the nitrogen, attached to the 3-position of an indole ring. The indole ring is further substituted at the 2-position with a (E)-3-phenylsulfonyl-2-propenyl group.	 Chemical structure of 1-methyl-2-((E)-3-phenylsulfonyl-2-propenyl)-1H-indole-3-ylpyrrolidine. It features a pyrrolidine ring with a methyl group on the nitrogen, attached to the 3-position of an indole ring. The indole ring is further substituted at the 2-position with a (E)-3-phenylsulfonyl-2-propenyl group.	EC number 430-560-5
191605-10-4	 Chemical structure of (2S,3S)-2-((4-methoxybenzoyl)oxy)-3-((4-methoxybenzoyl)oxy)butanedioic acid. It shows a central butanedioic acid chain with two 4-methoxybenzoyloxy groups attached at the 2 and 3 positions, both in the (S) configuration.	 Chemical structure of (2S,3S)-2-((4-methoxybenzoyl)oxy)-3-((4-methoxybenzoyl)oxy)butanedioic acid. It shows a central butanedioic acid chain with two 4-methoxybenzoyloxy groups attached at the 2 and 3 positions, both in the (S) configuration.	EC number 471-150-6
120807-02-5	 Chemical structure of (2S,3S)-2-((4-methoxybenzoyl)oxy)-3-((4-methoxybenzoyl)oxy)butanedioic acid. It shows a central butanedioic acid chain with two 4-methoxybenzoyloxy groups attached at the 2 and 3 positions, both in the (S) configuration.	 Chemical structure of (2S,3S)-2-((4-methoxybenzoyl)oxy)-3-((4-methoxybenzoyl)oxy)butanedioic acid. It shows a central butanedioic acid chain with two 4-methoxybenzoyloxy groups attached at the 2 and 3 positions, both in the (S) configuration.	EC number 416-040-0

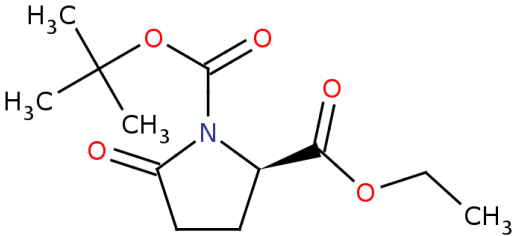
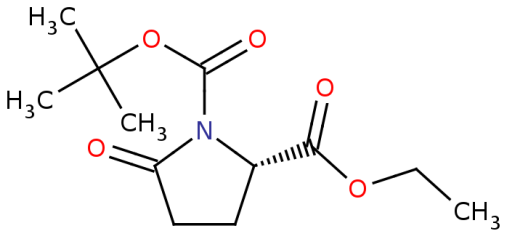
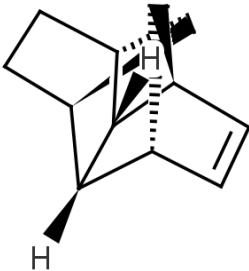
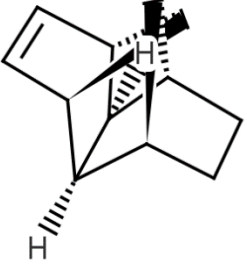
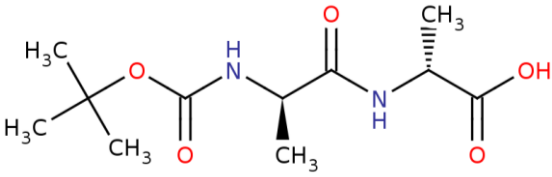
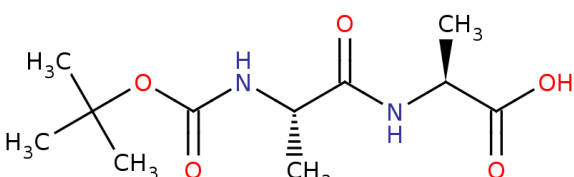
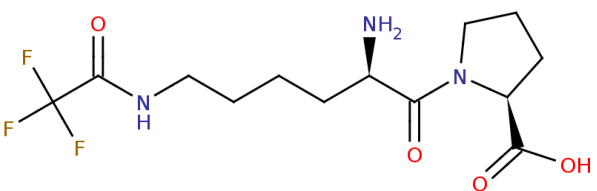
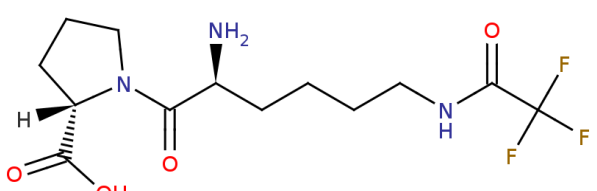
133855-98-8			EC number 406-850-2
156732-13-7			EC number 423-090-7
67914-85-6			EC number 267-747-4

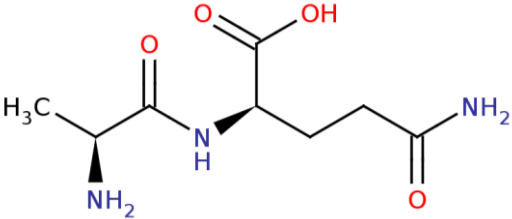
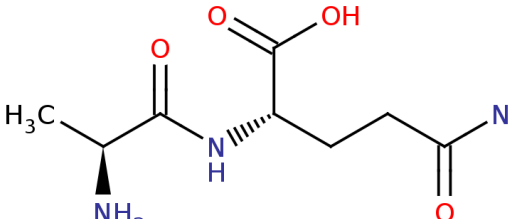
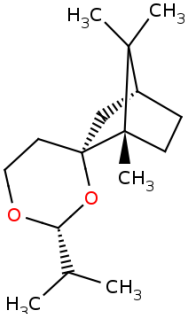
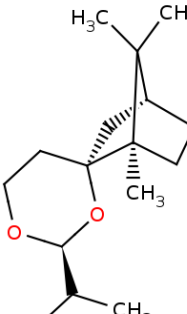
137590-32-0			EC number 415-820-8 both molecules differ
194602-27-2	HBr 	 HBr	EC number 421-810-4

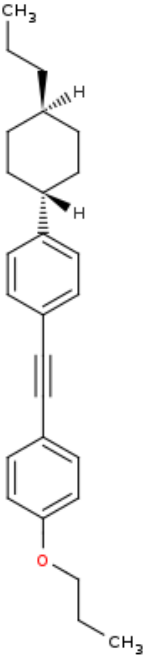
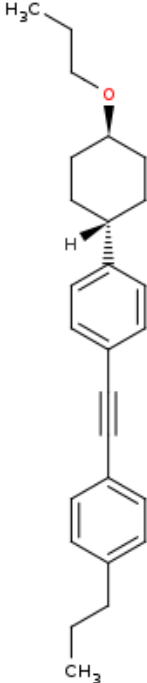
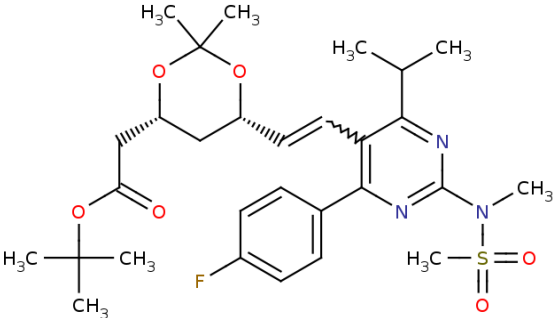
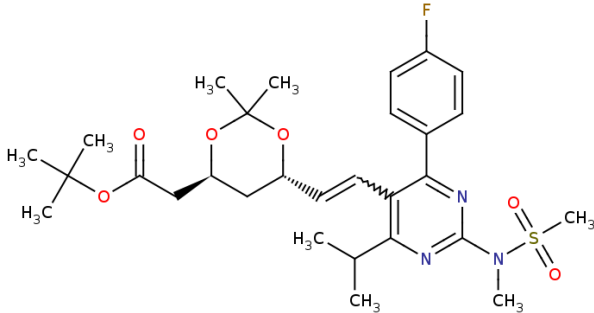
91465-08-6			EC number 415-130-7 the left molecule is different, the right molecule the same as the one in SciFinderⁿ
155661-07-7	HCl 	HCl 	EC number 445-550-6

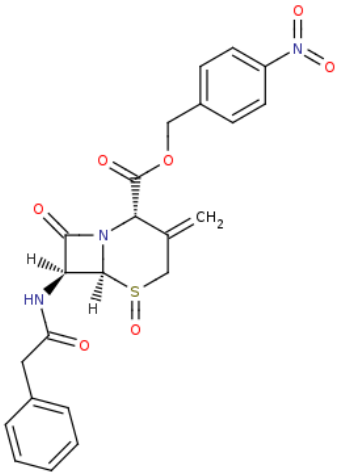
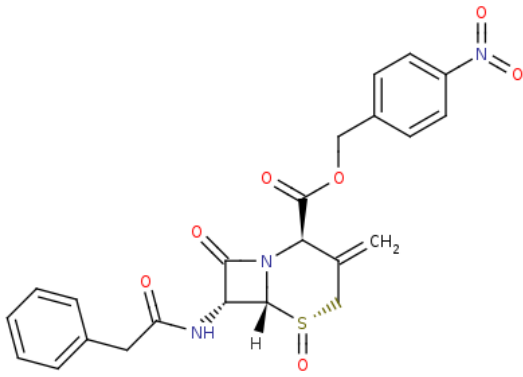
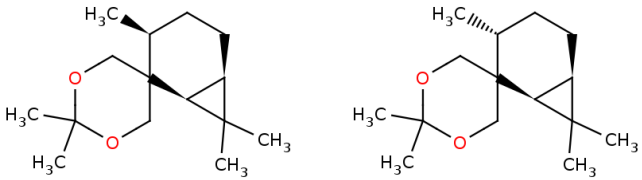
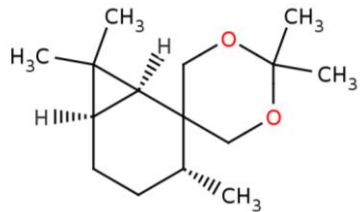
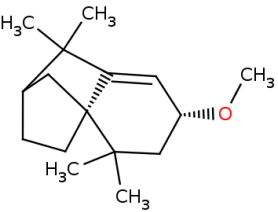
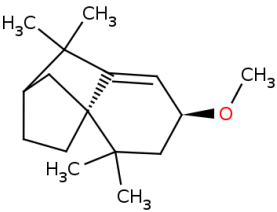
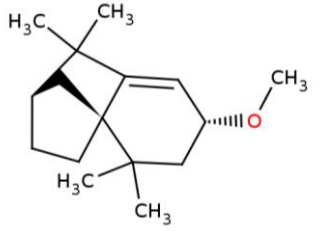
59653-74-6			EC number 423-400-0 both forms are in correct
793669-26-8			EC number 419-630-6 The CAS no. does not cover both forms. The left one is correct
167944-94-7			EC number 425-510-4

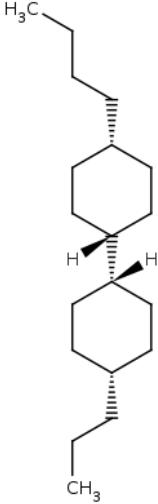
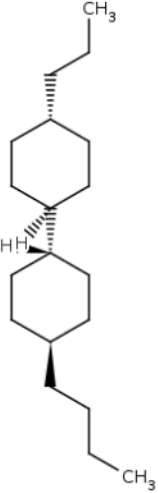
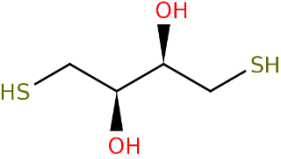
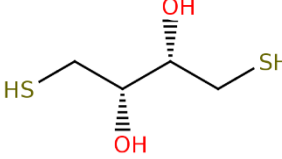
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125-12-2			EC number 204-727-6
150-86-7			EC number 416-120-5

144978-12-1			EC number 480-250-9
1076-12-6			EC number 700-678-4
27317-69-7			EC number 421-060-8
103300-89-6			EC number 402-920-1

39537-23-0	 Chemical structure of (S)-2-amino-3-((S)-2-amino-3-oxopropyl)butanoic acid. The structure shows a central chiral center (C2) bonded to a carboxylic acid group (COOH), an amino group (NH2), and a 3-oxopropyl chain. The amino group is on a wedge, and the 3-oxopropyl chain is on a dash.	 Chemical structure of (R)-2-amino-3-((S)-2-amino-3-oxopropyl)butanoic acid. The structure is identical to the previous one, but the amino group is on a dash and the 3-oxopropyl chain is on a wedge.	EC number 475-290-9
188199-50-0	 Chemical structure of (1S,2S,3S,4S)-1,2,3,4-tetrahydro-2H-pyran-2-yl 2,3-dimethylbutyrate. The structure shows a tetrahydropyran ring with a methyl group at C2 (wedge), a 2,3-dimethylbutyrate ester group at C3 (wedge), and a methyl group at C4 (wedge).	 Chemical structure of (1R,2R,3R,4R)-1,2,3,4-tetrahydro-2H-pyran-2-yl 2,3-dimethylbutyrate. The structure is identical to the previous one, but the methyl group at C2 is on a dash, the 2,3-dimethylbutyrate ester group at C3 is on a dash, and the methyl group at C4 is on a dash.	EC number 443-460-1

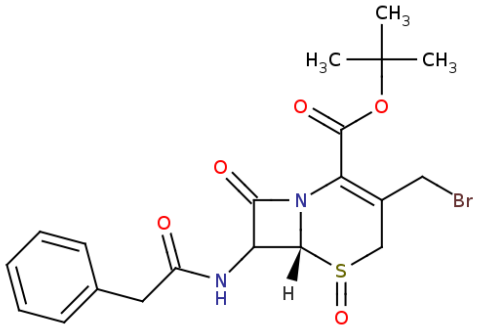
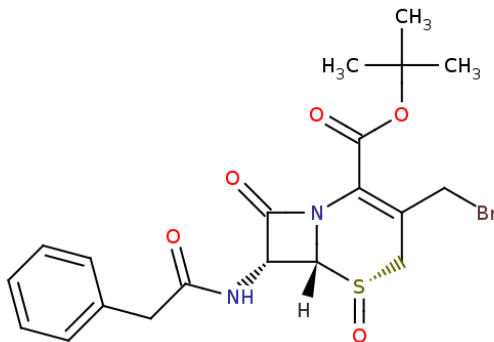
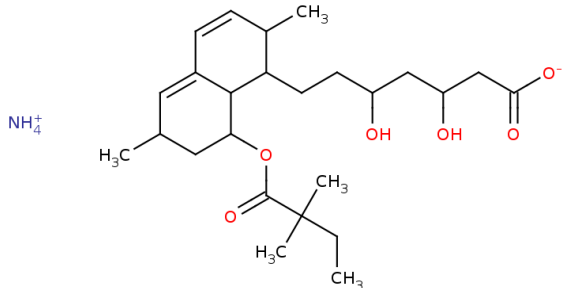
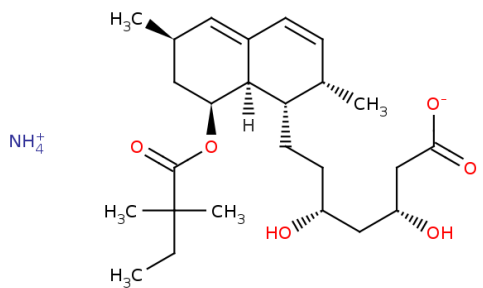
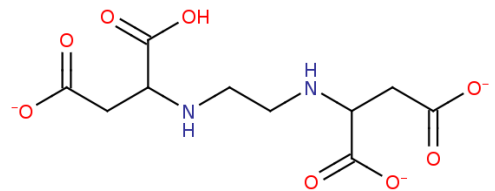
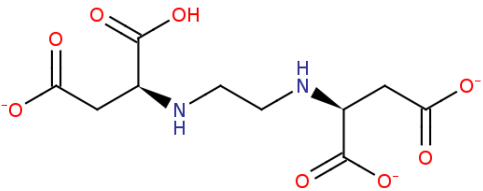
348113-98-4	 Chemical structure of 1-((4-((4-ethoxyphenyl)ethynyl)phenyl)phenyl)ethanol. It features a central benzene ring connected via a triple bond to a para-substituted phenyl ring with an ethoxy group (-OCH₂CH₂CH₃). The central ring is also connected via a double bond to another para-substituted phenyl ring, which is further connected to a 1-ethoxyethyl group (-CH(OH)CH₂CH₂CH₃).	 Chemical structure of 1-((4-((4-ethoxyphenyl)ethynyl)phenyl)phenyl)ethanol. It features a central benzene ring connected via a triple bond to a para-substituted phenyl ring with an ethoxy group (-OCH₂CH₂CH₃). The central ring is also connected via a double bond to another para-substituted phenyl ring, which is further connected to a 1-ethoxyethyl group (-CH(OH)CH₂CH₂CH₃).	EC number 448-430-1
1379976-09-6	 Chemical structure of 1-((4-((4-((4-ethoxyphenyl)ethynyl)phenyl)phenyl)ethoxy)phenyl)ethanol. It features a central benzene ring connected via a triple bond to a para-substituted phenyl ring with an ethoxy group (-OCH₂CH₂CH₃). The central ring is also connected via a double bond to another para-substituted phenyl ring, which is further connected to a 1-ethoxyethyl group (-CH(OH)CH₂CH₂CH₃).	 Chemical structure of 1-((4-((4-((4-ethoxyphenyl)ethynyl)phenyl)phenyl)ethoxy)phenyl)ethanol. It features a central benzene ring connected via a triple bond to a para-substituted phenyl ring with an ethoxy group (-OCH₂CH₂CH₃). The central ring is also connected via a double bond to another para-substituted phenyl ring, which is further connected to a 1-ethoxyethyl group (-CH(OH)CH₂CH₂CH₃).	EC number 432-810-9

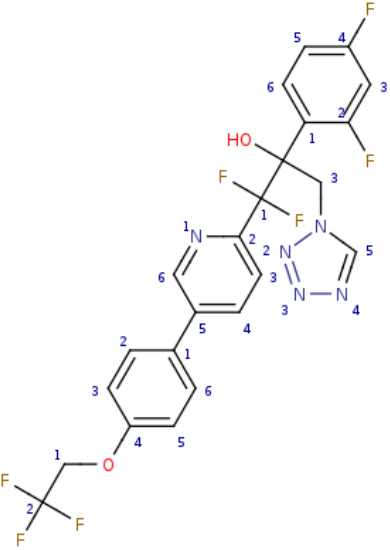
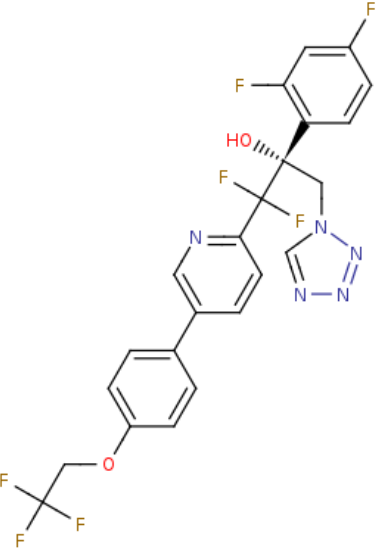
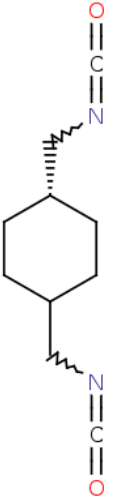
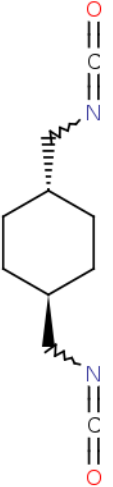
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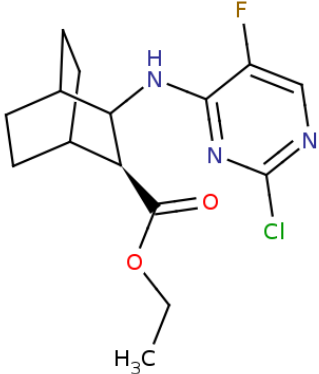
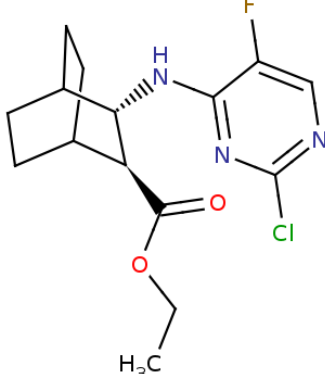
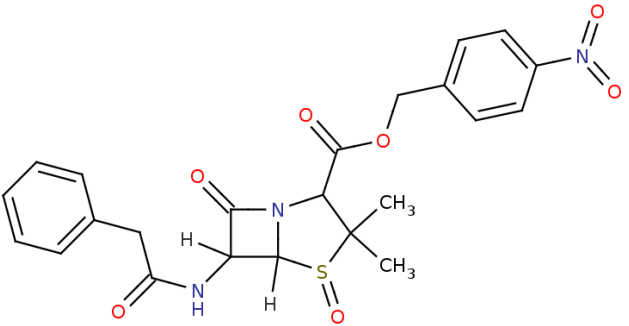
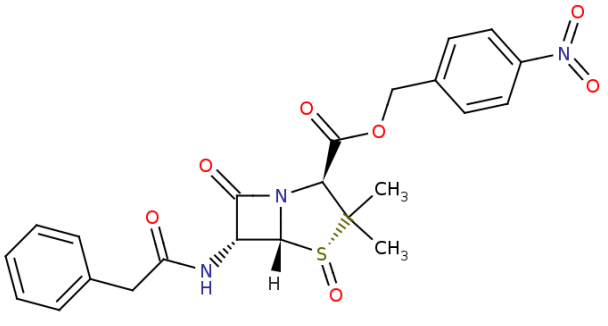
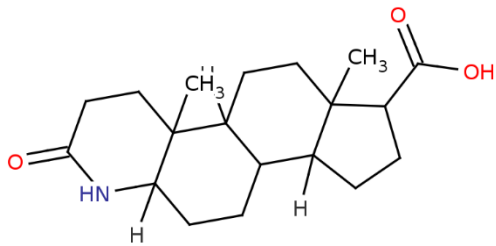
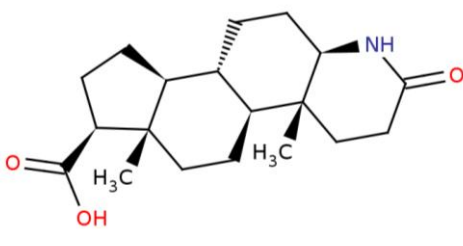
96624-52-1	 Chemical structure of 1,4-bis(4-propylphenyl)-2,3-dihydro-1,4-dioxane. It features a central 1,4-dioxane ring with two propylphenyl groups attached at the 1 and 4 positions. The propyl groups are labeled H₃C and CH₃.	 Chemical structure of 1,4-bis(4-propylphenyl)-2,3-dihydro-1,4-dioxane. It features a central 1,4-dioxane ring with two propylphenyl groups attached at the 1 and 4 positions. The propyl groups are labeled CH₃.	EC number 619-232-4
3483-12-3	 Chemical structure of 2,4-dithiolanediol. It is a five-membered ring with two sulfur atoms (SH) and two hydroxyl groups (OH). The hydroxyl groups are shown with wedge and dash bonds.	 Chemical structure of 2,4-dithiolanediol. It is a five-membered ring with two sulfur atoms (SH) and two hydroxyl groups (OH). The hydroxyl groups are shown with wedge and dash bonds.	EC number 222-468-7

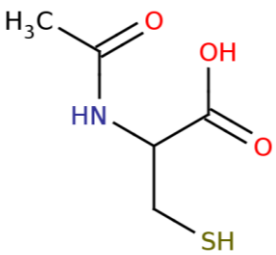
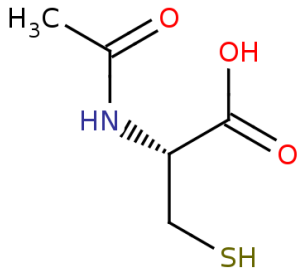
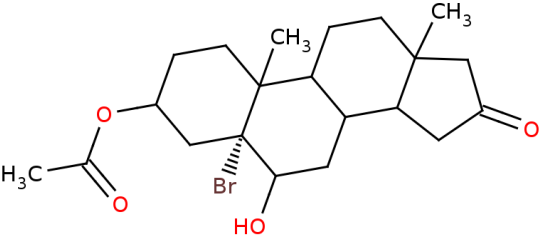
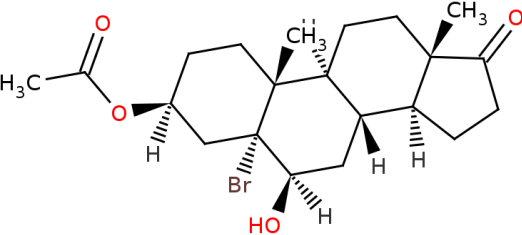
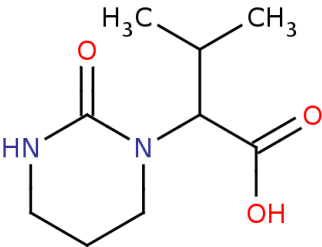
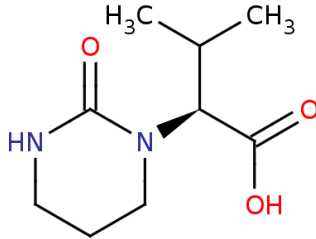
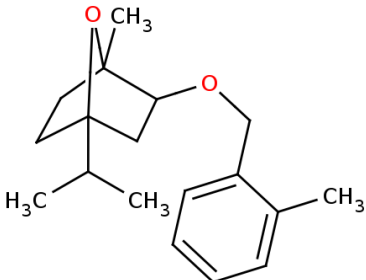
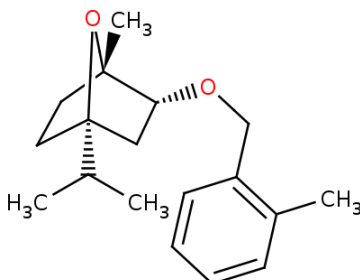
6) Inconsistencies related to the stereochemistry (no stereochemistry information in the ECHA database while SciFinderⁿ has some)

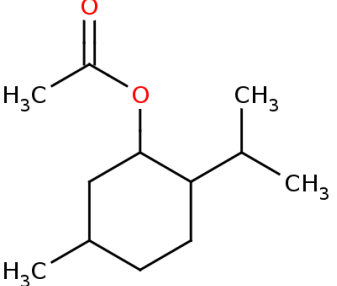
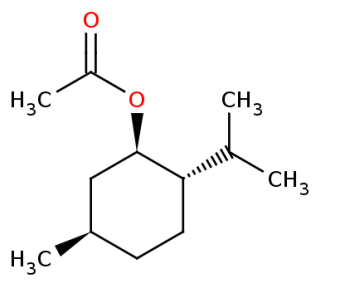
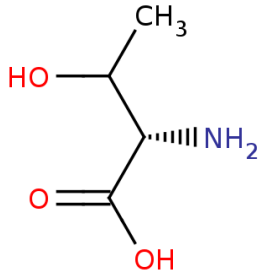
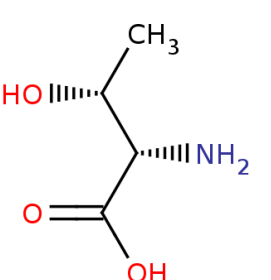
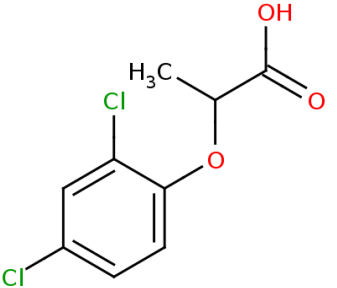
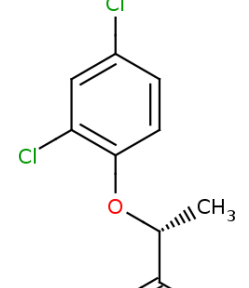
Table 6: Substances in the ECHA database where the SMILES do not correspond to the CAS RNTM as allocated in SciFindern. The reason for the mismatches here are stereochemistry information that are not available in the ECHA database while SciFindern has some.

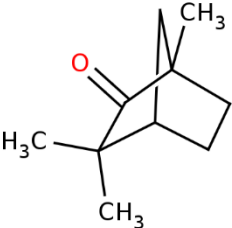
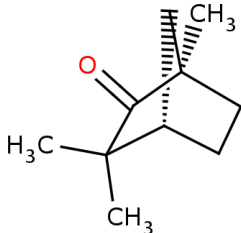
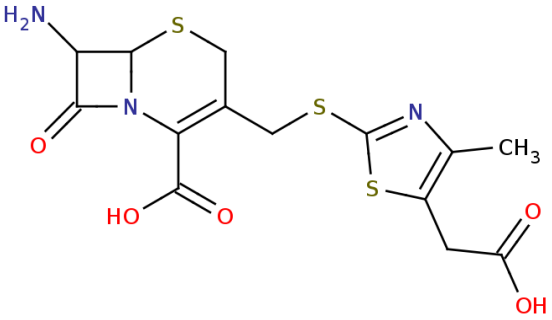
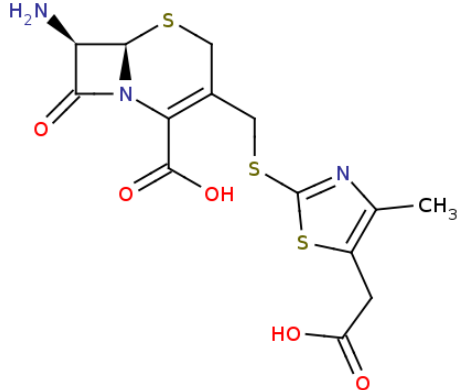
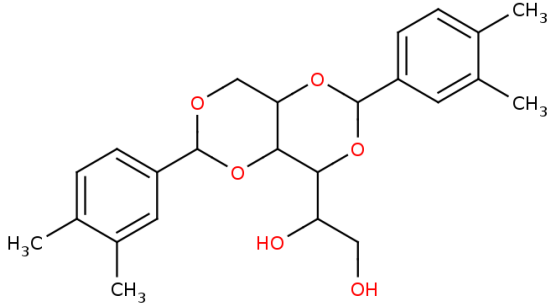
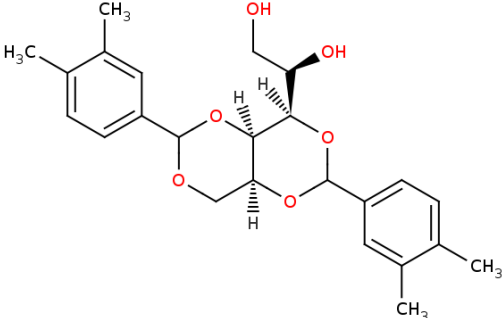
CAS RN TM	Structure in the database	Structure corresponding to the CAS RN TM	Comment
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139893-43-9			EC number 404-520-2
178949-82-1	Na ⁺ Na ⁺ Na ⁺ 	Na ⁺ Na ⁺ Na ⁺ 	EC number 416-530-4

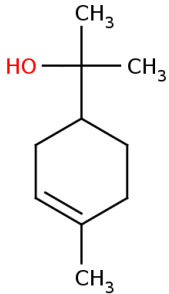
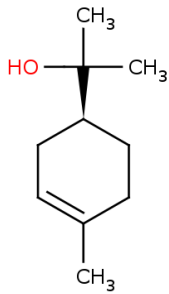
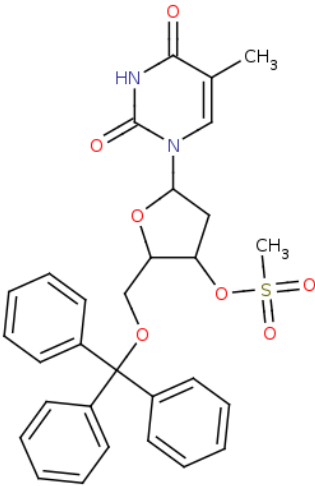
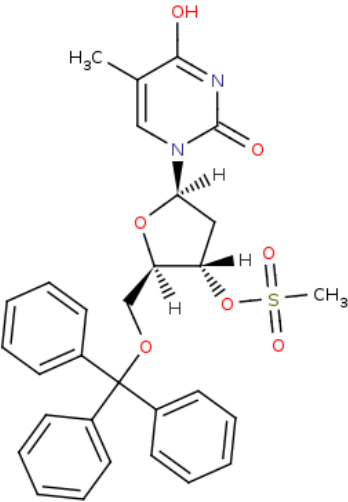
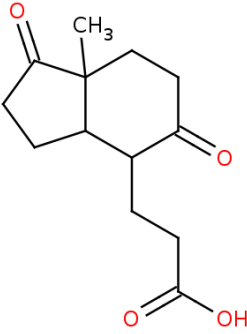
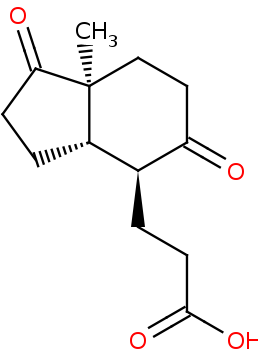
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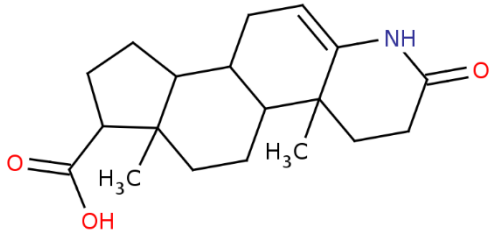
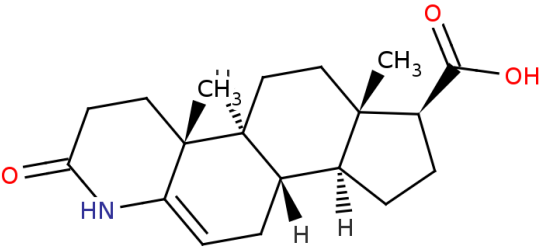
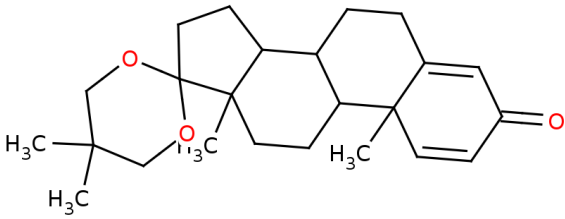
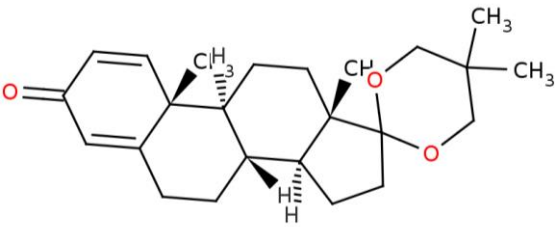
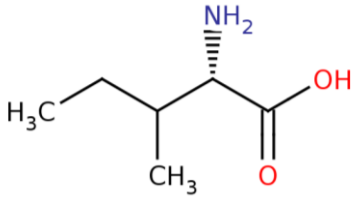
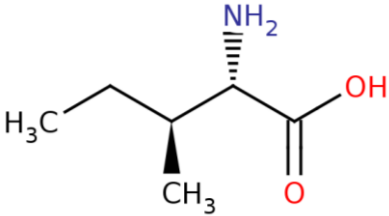
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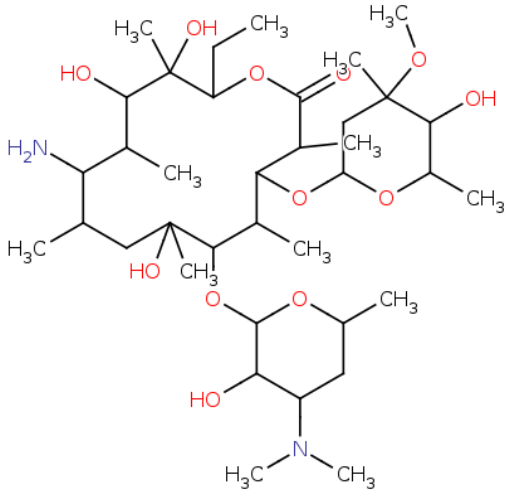
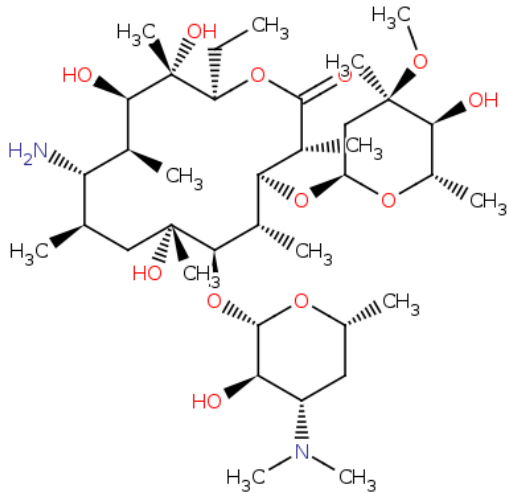
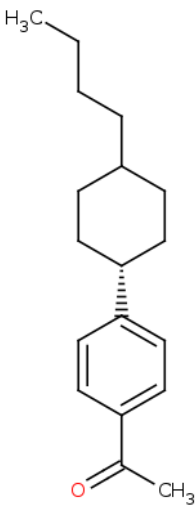
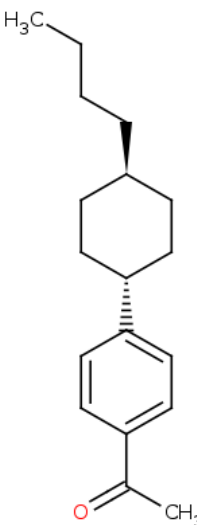
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192725-50-1	 <chem>CC(C)C(C(=O)O)N1CCCCN1C2=CC=CC=C2</chem>	 <chem>CC(C)C(C(=O)O)[C@H]1CCNCC1N2=CC=CC=C2</chem>	EC number 430-900-2
87818-31-3	 <chem>CC1(C)CC2C(C1)C(=O)CC3C2(C)CC(C3)C4BrO</chem>	 <chem>CC1(C)CC2C(C1)C(=O)CC3C2(C)CC(C3)C4BrO</chem>	EC number 402-410-9

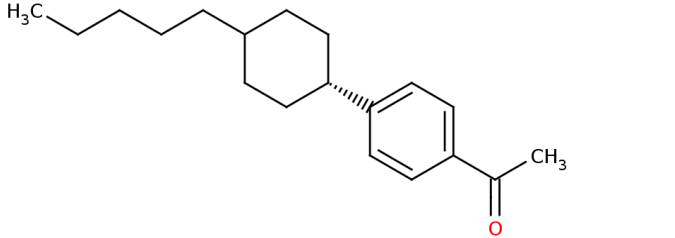
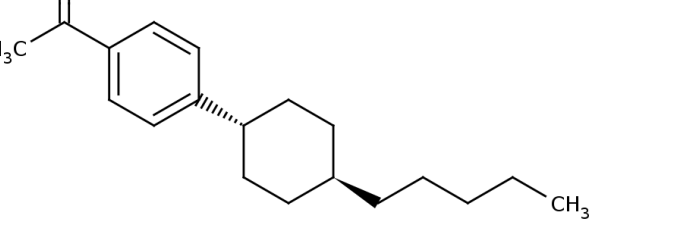
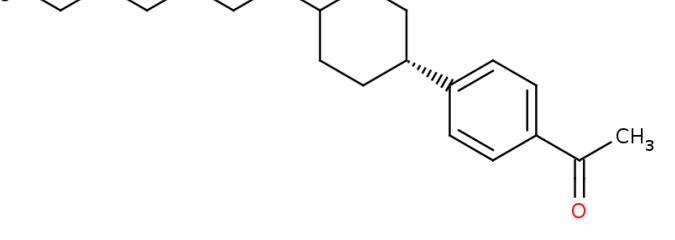
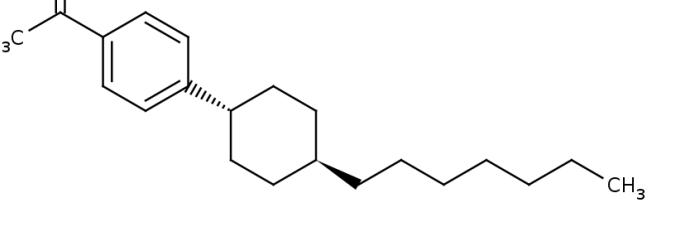
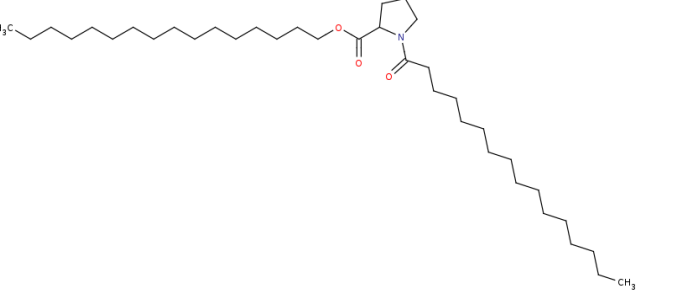
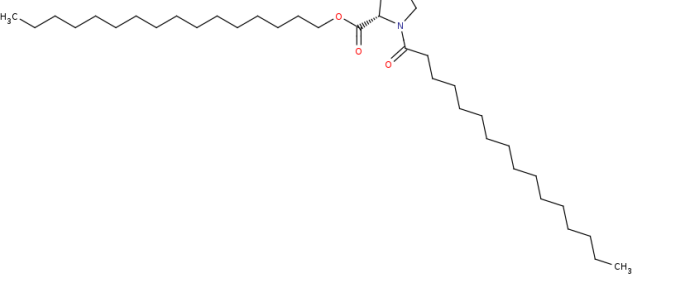
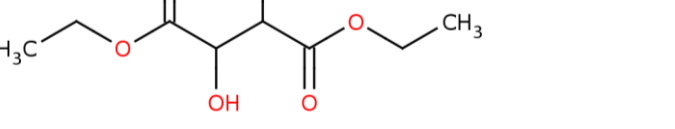
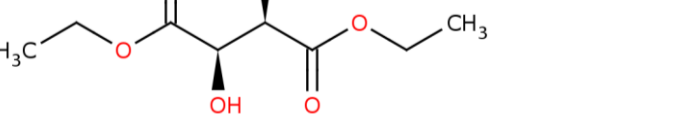
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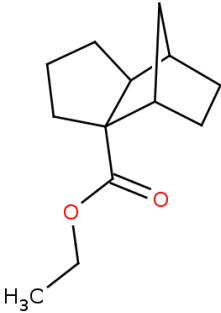
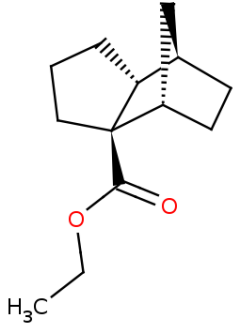
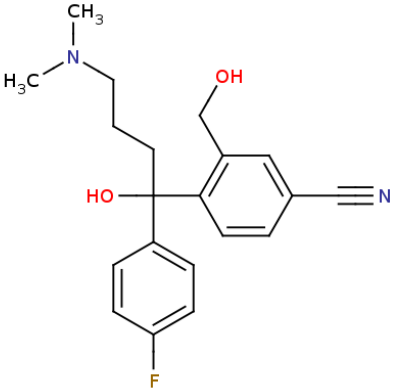
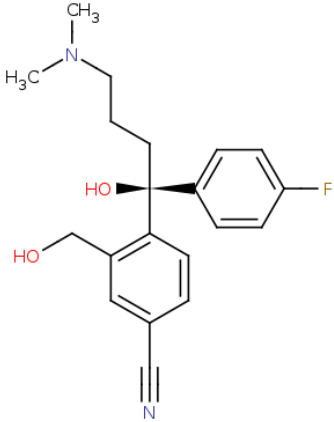
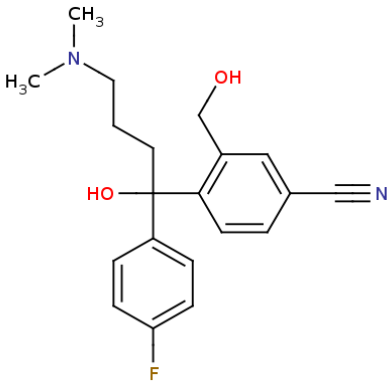
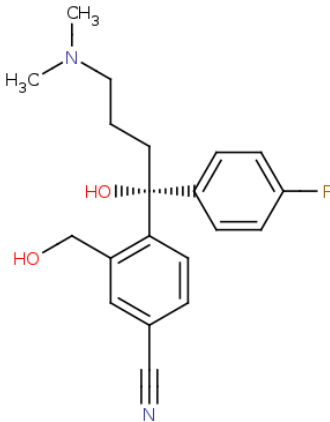
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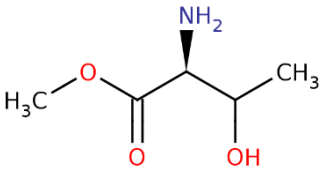
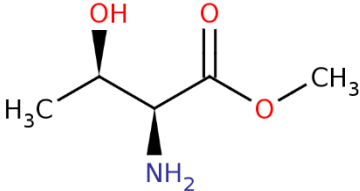
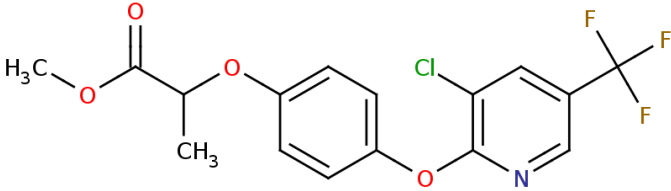
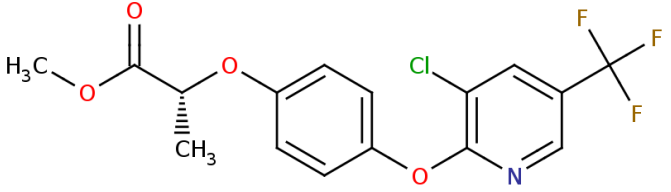
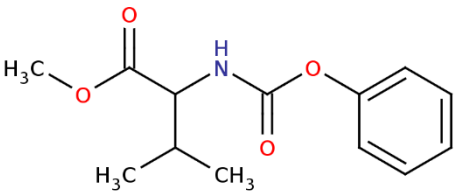
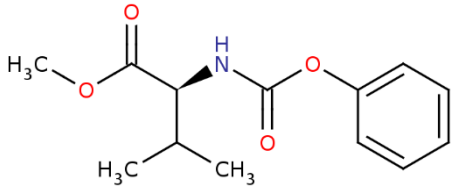
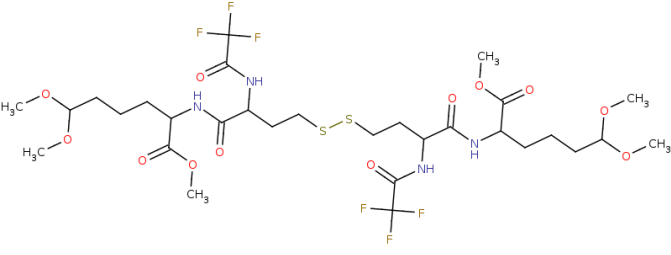
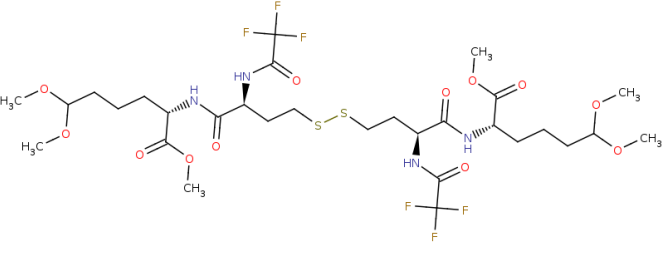
10482-56-1	 Chemical structure of 2-(4-methylcyclohex-2-en-1-yl)-2-methylpropan-1-ol. It features a cyclohexene ring with a methyl group at the 4-position and a 2-methylpropan-1-ol group at the 1-position. The hydroxyl group is highlighted in red.	 Chemical structure of (S)-2-(4-methylcyclohex-2-en-1-yl)-2-methylpropan-1-ol. It features a cyclohexene ring with a methyl group at the 4-position and a 2-methylpropan-1-ol group at the 1-position. The hydroxyl group is highlighted in red, and the stereochemistry at the chiral center is (S).	EC number 233-986-8
104218-44-2	 Chemical structure of 1-(4-methyl-2-oxo-1,2,3,4-tetrahydropyrimidin-5-yl)-2-(benzoyloxy)methyl-2-phenyl-1,3-dioxolane-5-sulfonate. It features a pyrimidine ring with a methyl group at the 4-position and a 1,3-dioxolane ring at the 5-position. The dioxolane ring is substituted with a benzoyloxy group and a methylsulfonate group. The hydroxyl group in the pyrimidine ring is highlighted in red.	 Chemical structure of (S)-1-(4-methyl-2-oxo-1,2,3,4-tetrahydropyrimidin-5-yl)-2-(benzoyloxy)methyl-2-phenyl-1,3-dioxolane-5-sulfonate. It features a pyrimidine ring with a methyl group at the 4-position and a 1,3-dioxolane ring at the 5-position. The dioxolane ring is substituted with a benzoyloxy group and a methylsulfonate group. The hydroxyl group in the pyrimidine ring is highlighted in red, and the stereochemistry at the chiral center is (S).	EC number 406-360-9
1944-63-4	 Chemical structure of 2-(4-methyl-2-oxo-1,2,3,4-tetrahydropyrimidin-5-yl)-2-(benzoyloxy)methyl-2-phenyl-1,3-dioxolane-5-sulfonate. It features a pyrimidine ring with a methyl group at the 4-position and a 1,3-dioxolane ring at the 5-position. The dioxolane ring is substituted with a benzoyloxy group and a methylsulfonate group. The hydroxyl group in the pyrimidine ring is highlighted in red.	 Chemical structure of (S)-2-(4-methyl-2-oxo-1,2,3,4-tetrahydropyrimidin-5-yl)-2-(benzoyloxy)methyl-2-phenyl-1,3-dioxolane-5-sulfonate. It features a pyrimidine ring with a methyl group at the 4-position and a 1,3-dioxolane ring at the 5-position. The dioxolane ring is substituted with a benzoyloxy group and a methylsulfonate group. The hydroxyl group in the pyrimidine ring is highlighted in red, and the stereochemistry at the chiral center is (S).	EC number 435-830-6

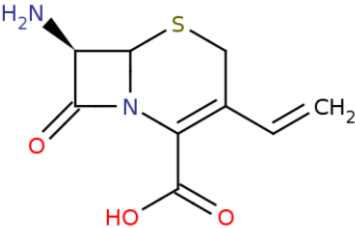
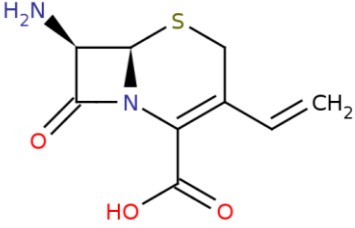
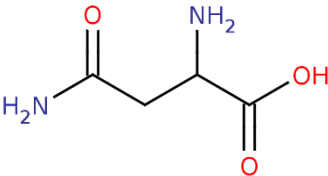
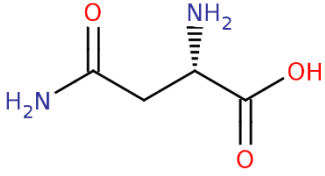
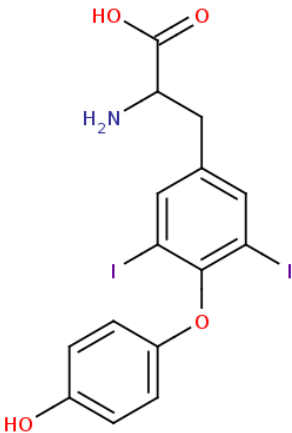
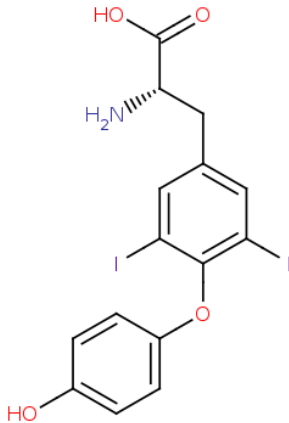
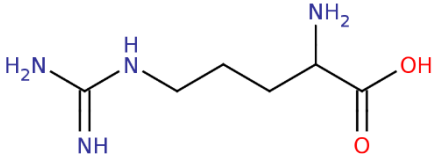
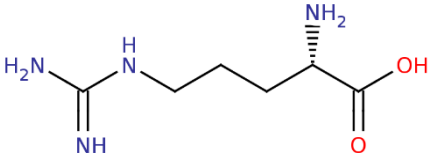
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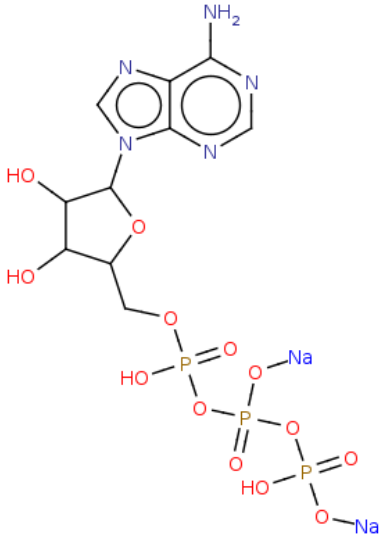
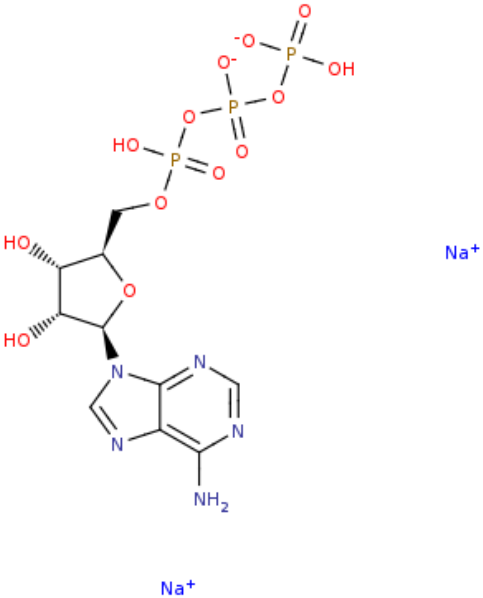
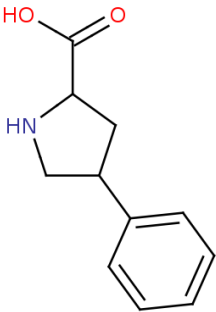
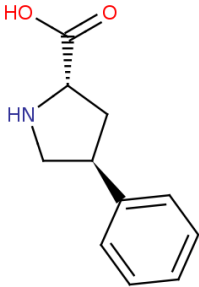
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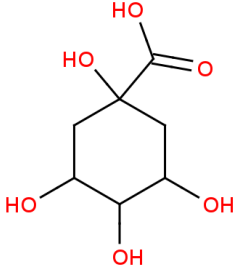
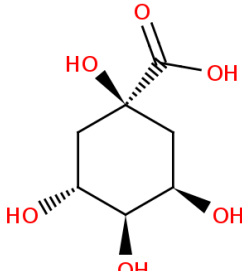
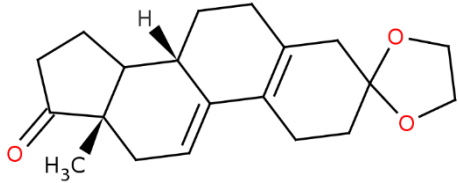
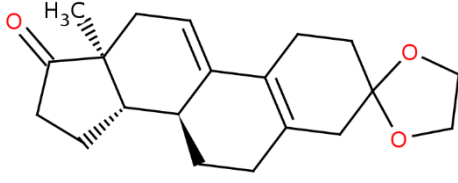
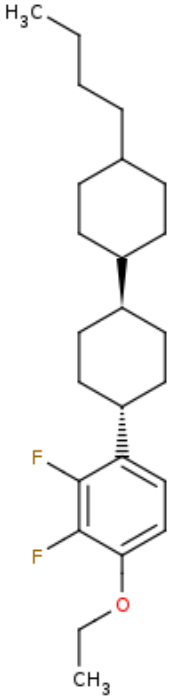
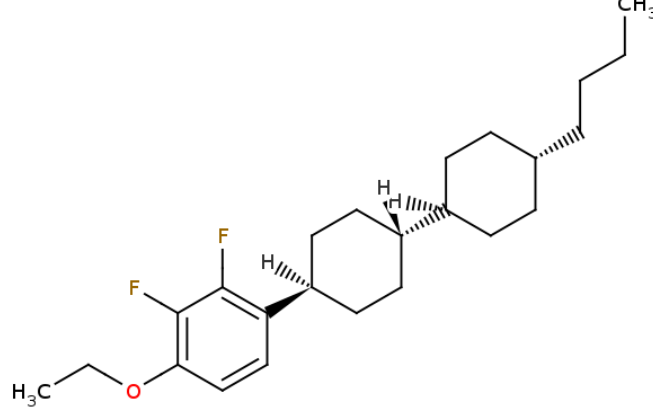
78531-59-6	 Chemical structure of 4-(4-(4-oxopentyl)cyclohexyl)benzoic acid. It features a cyclohexane ring substituted with a 4-oxopentyl group and a 4-(4-cyclohexylbenzoyl) group.	 Chemical structure of 4-(4-(4-oxopentyl)cyclohexyl)benzoic acid. It features a cyclohexane ring substituted with a 4-oxopentyl group and a 4-(4-cyclohexylbenzoyl) group.	EC number 426-830-7
78531-60-9	 Chemical structure of 4-(4-(4-oxopentyl)cyclohexyl)benzoic acid. It features a cyclohexane ring substituted with a 4-oxopentyl group and a 4-(4-cyclohexylbenzoyl) group.	 Chemical structure of 4-(4-(4-oxopentyl)cyclohexyl)benzoic acid. It features a cyclohexane ring substituted with a 4-oxopentyl group and a 4-(4-cyclohexylbenzoyl) group.	EC number 426-820-2
791838-11-4	 Chemical structure of 1-(4-(4-oxopentyl)cyclohexyl)benzoic acid. It features a cyclohexane ring substituted with a 4-oxopentyl group and a 4-(4-cyclohexylbenzoyl) group.	 Chemical structure of 1-(4-(4-oxopentyl)cyclohexyl)benzoic acid. It features a cyclohexane ring substituted with a 4-oxopentyl group and a 4-(4-cyclohexylbenzoyl) group.	EC number 479-990-5
87-91-2	 Chemical structure of 1,2-bis(4-oxopentyl)-1,2-ethanediol. It features a central ethane-1,2-diol moiety substituted with two 4-oxopentyl groups.	 Chemical structure of 1,2-bis(4-oxopentyl)-1,2-ethanediol. It features a central ethane-1,2-diol moiety substituted with two 4-oxopentyl groups.	EC number 201-783-3

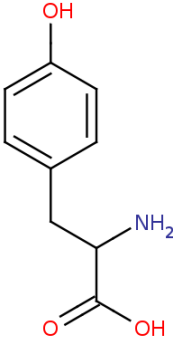
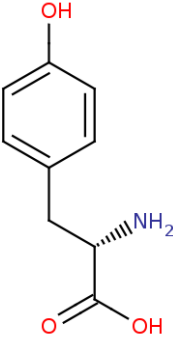
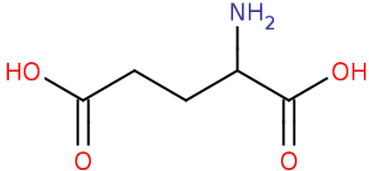
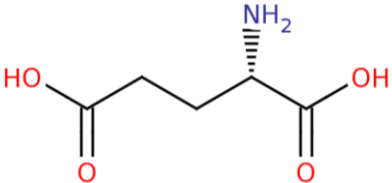
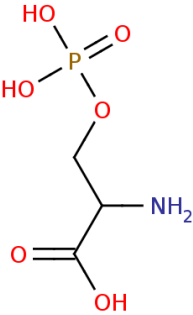
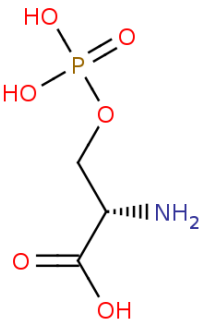
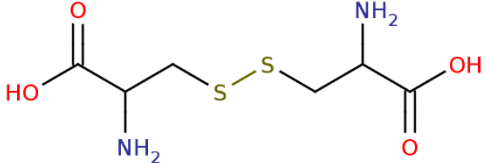
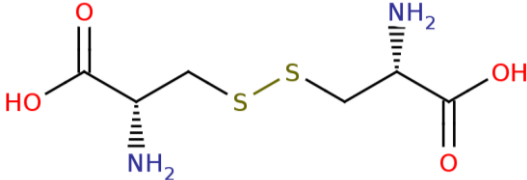
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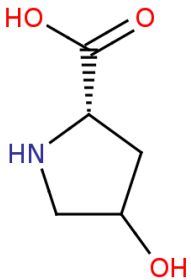
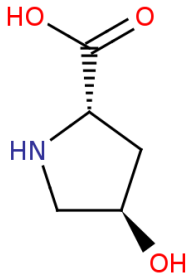
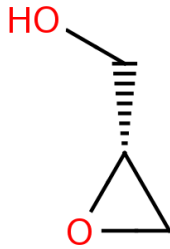
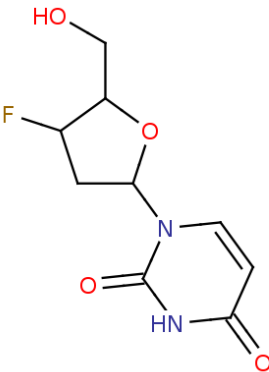
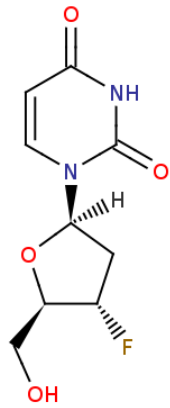
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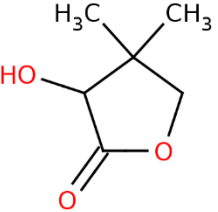
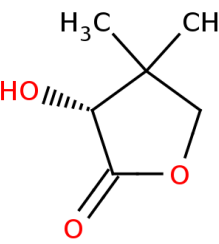
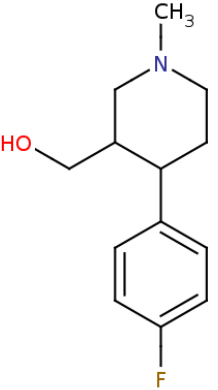
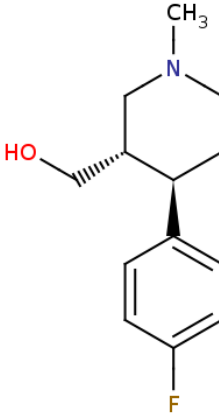
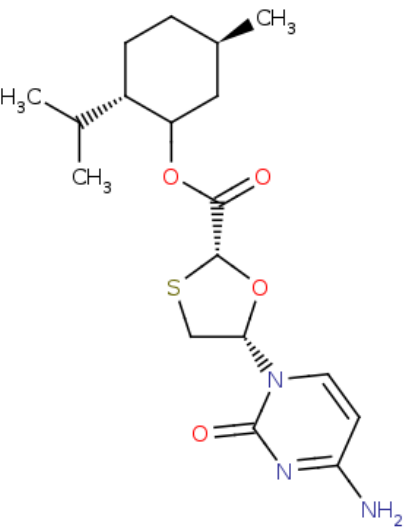
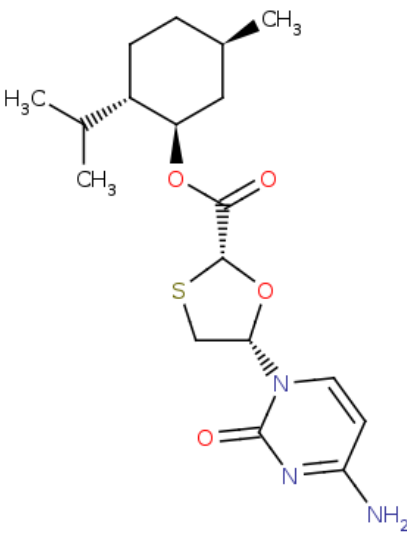
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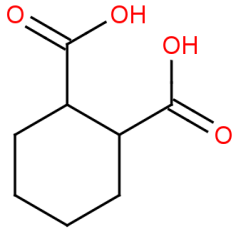
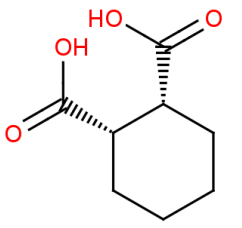
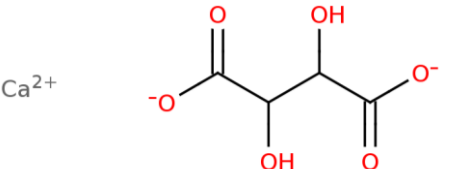
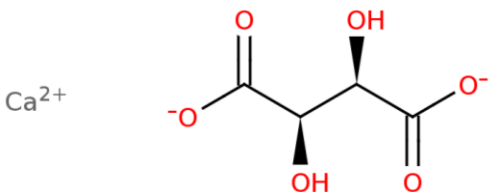
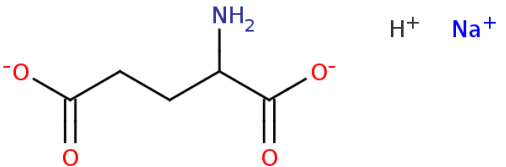
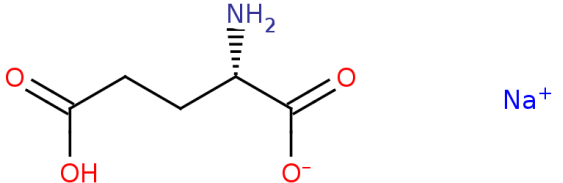
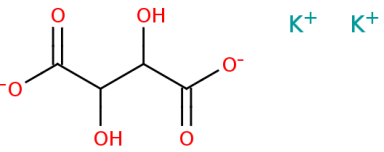
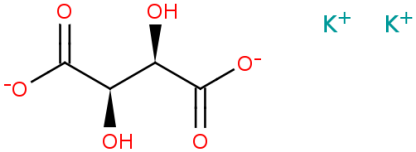
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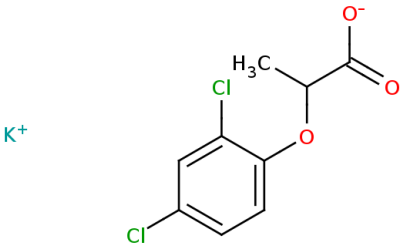
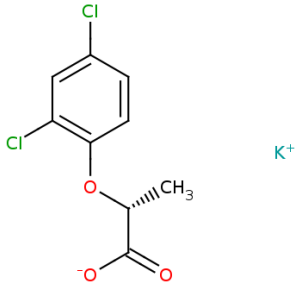
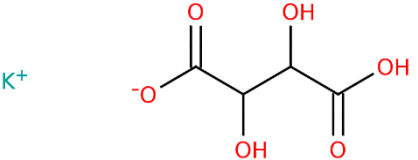
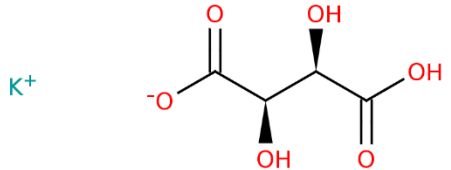
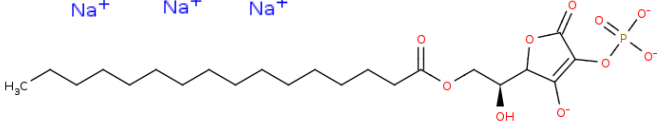
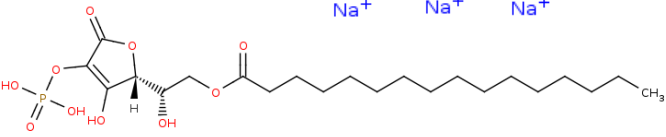
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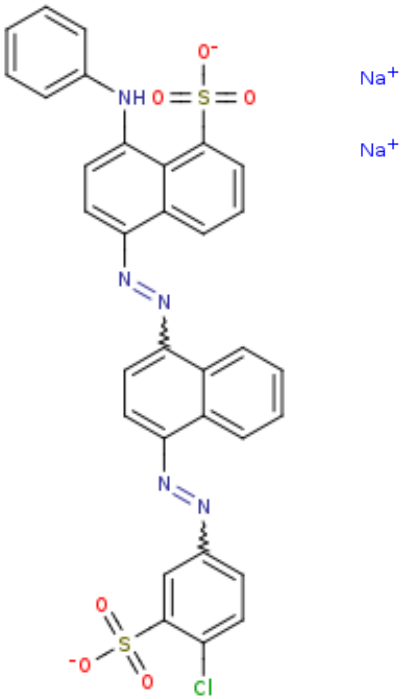
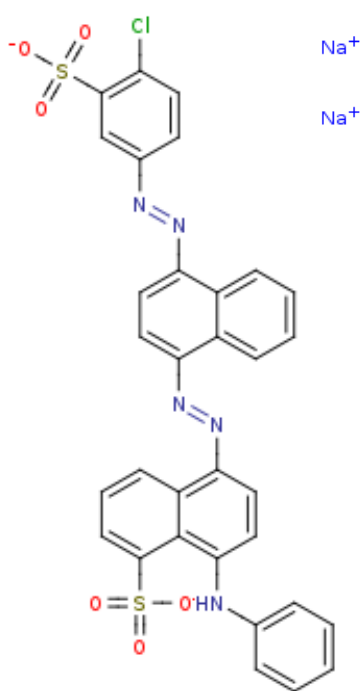
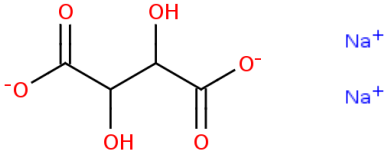
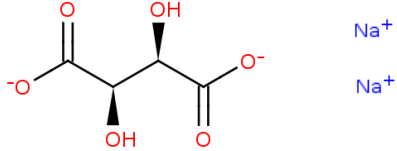
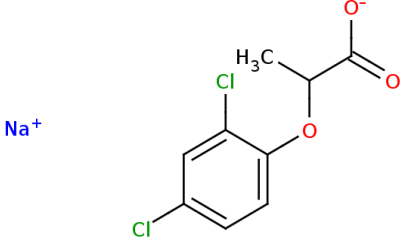
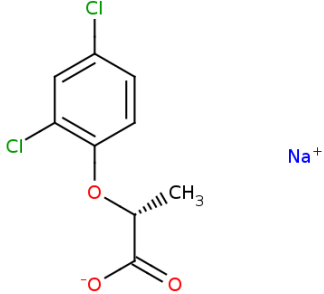
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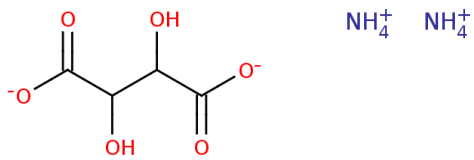
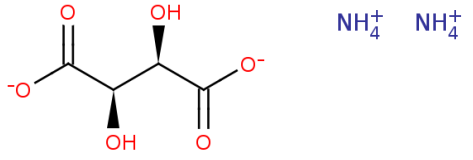
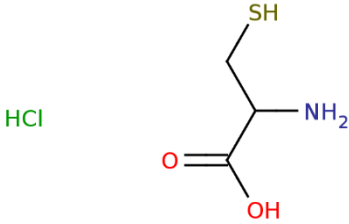
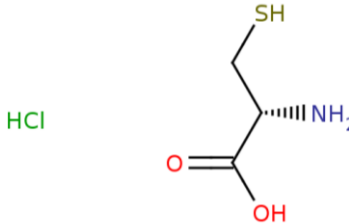
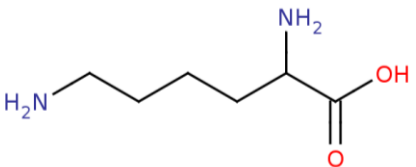
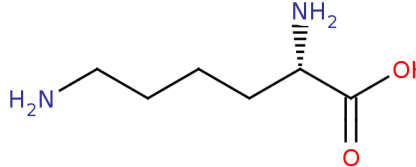
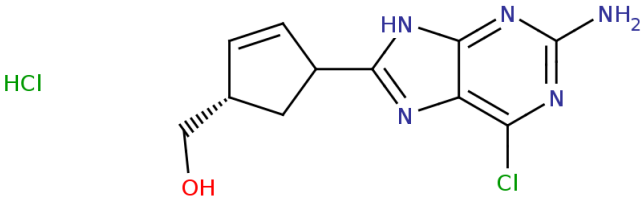
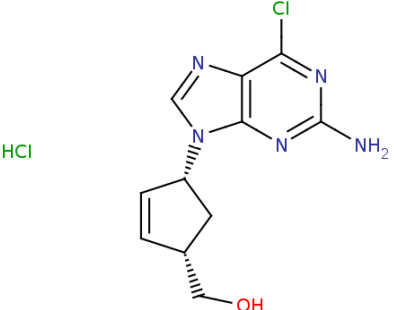
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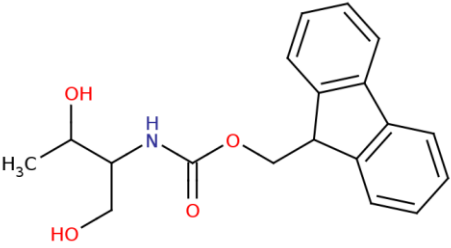
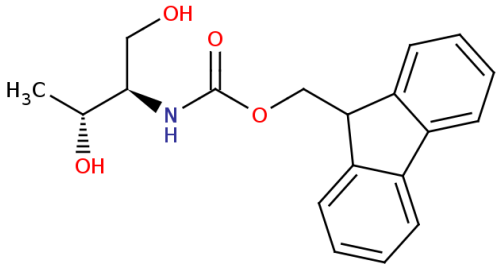
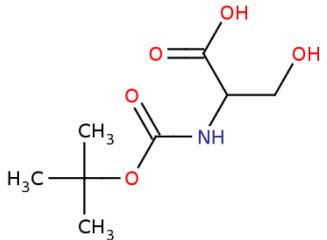
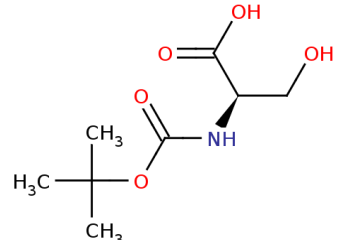
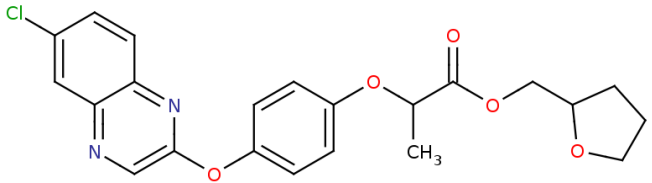
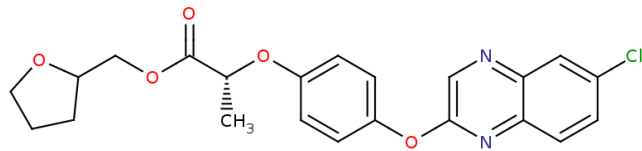
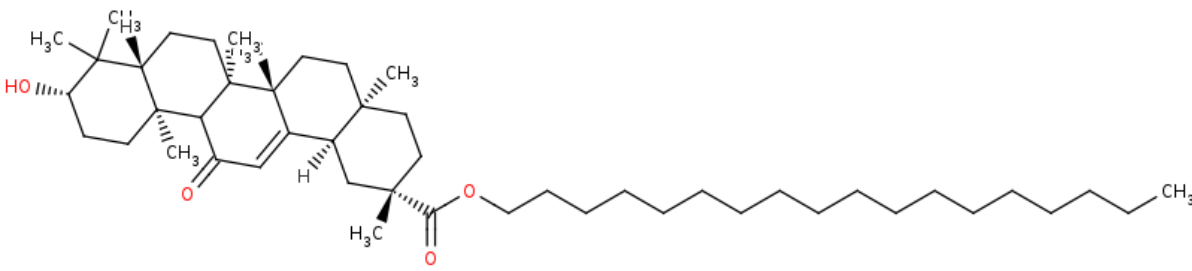
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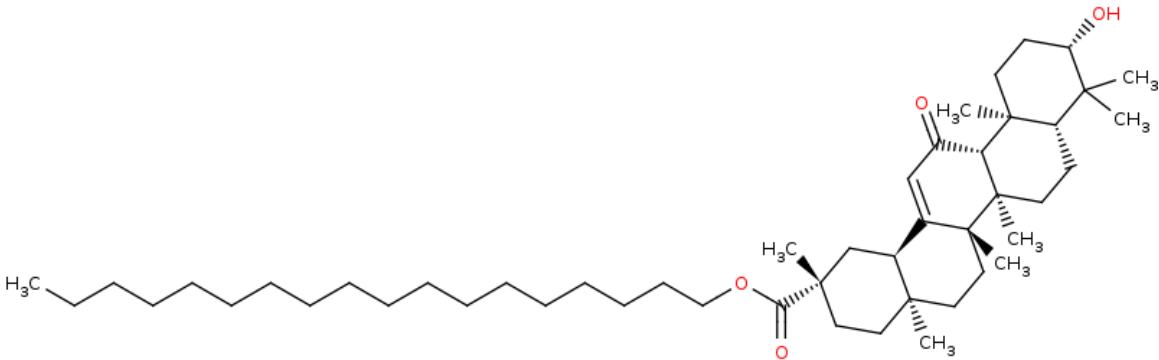
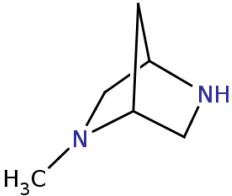
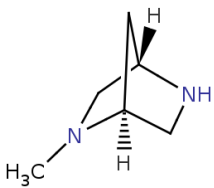
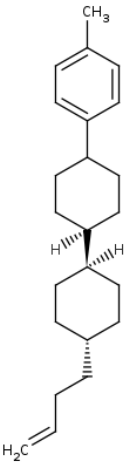
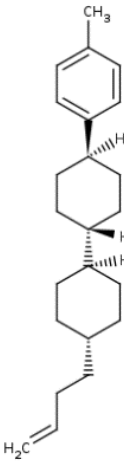
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3164-34-9			EC number 221-621-5
142-47-2			EC number 205-538-1
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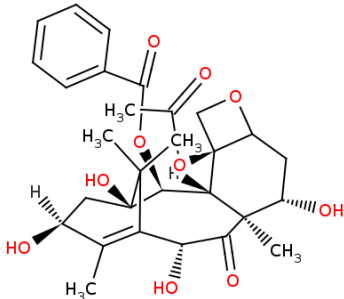
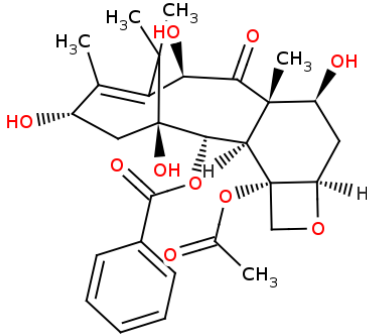
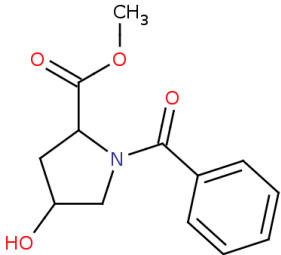
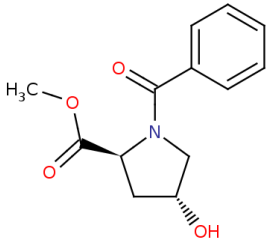
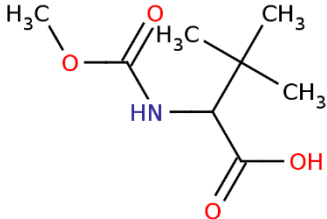
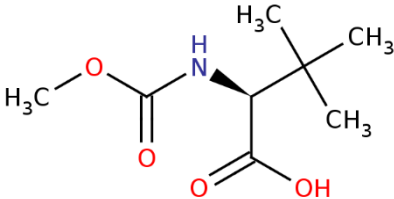
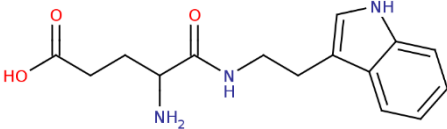
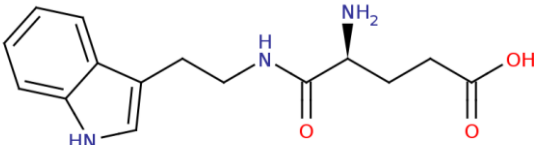
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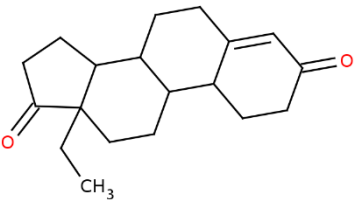
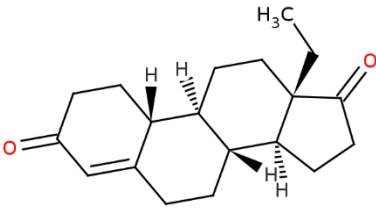
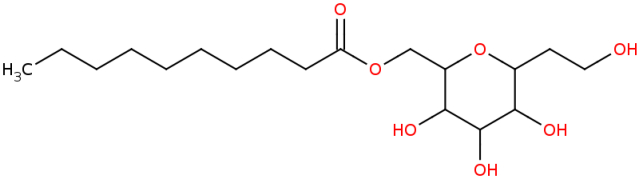
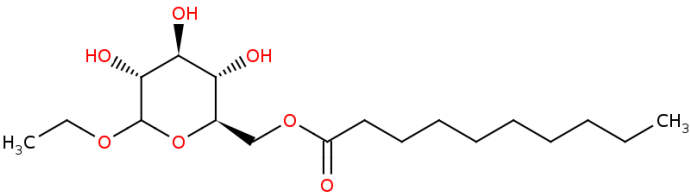
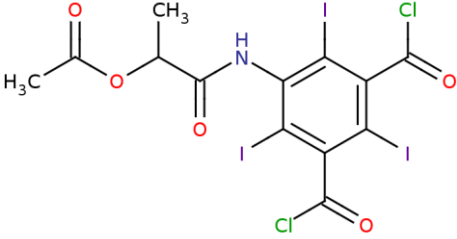
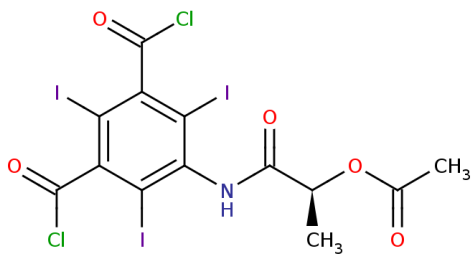
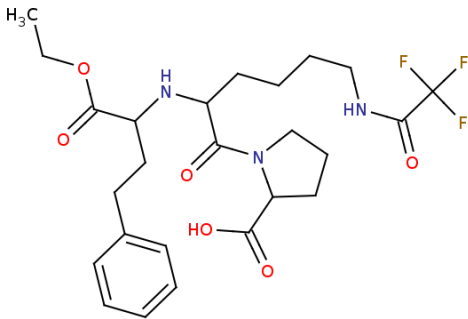
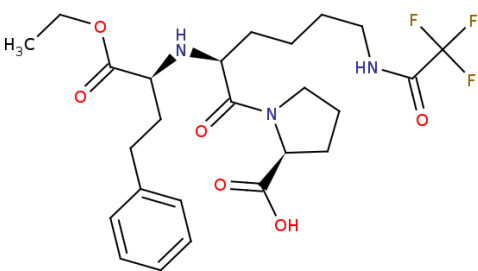
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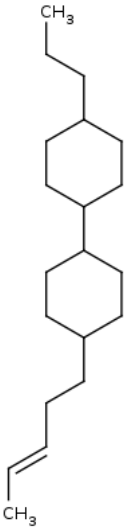
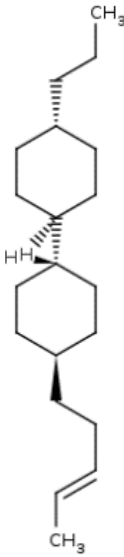
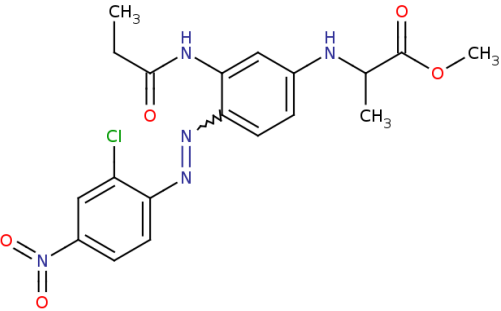
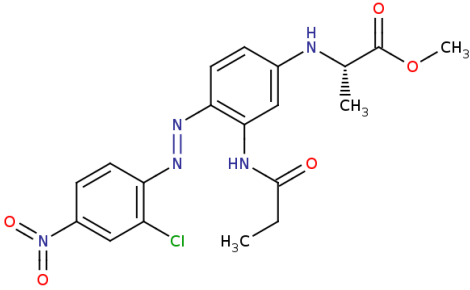
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657-27-2			EC number 211-519-9
172015-79-1			EC number 426-200-1

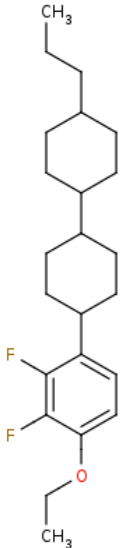
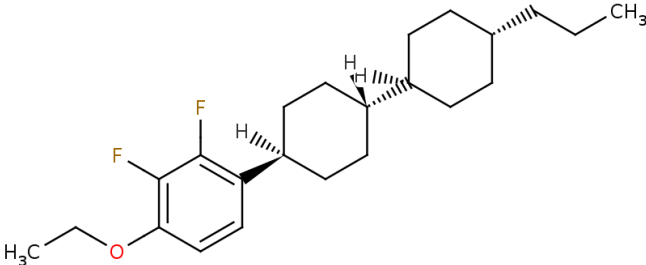
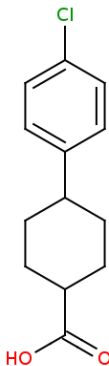
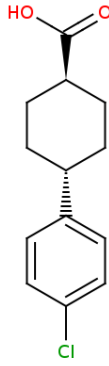
176380-53-3			EC number 439-410-3
6368-20-3			EC number 444-670-6
200509-41-7			EC number 414-200-4
13832-70-7 (incorrect)			EC number 419-580-5

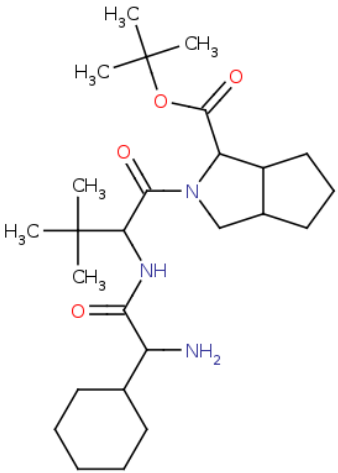
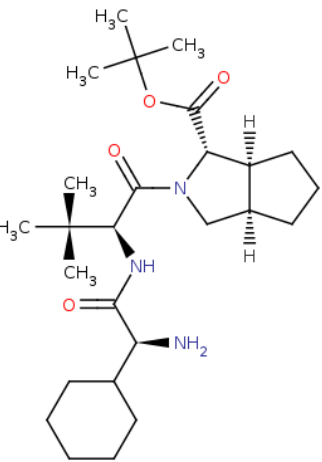
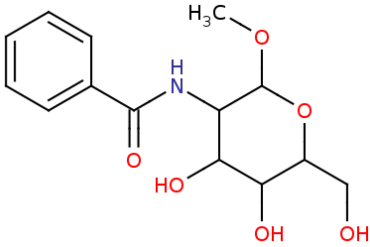
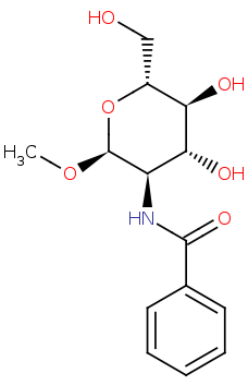
13832-70-7 (correct)	 The structure shows a steroid nucleus with a long alkyl chain (H₃C-(CH₂)₁₈-O-) attached to the 3-position. The steroid has a hydroxyl group (OH) at C-3, a methyl group (CH₃) at C-10, and a methyl group (CH₃) at C-13. The stereochemistry is indicated with wedges and dashes.		EC number 419-580-5
125224-62-6	 The structure shows a bicyclic amine derivative with a methyl group (H₃C) attached to the nitrogen atom. The stereochemistry is indicated with wedges and dashes. HBr HBr	 The structure shows a bicyclic amine derivative with a methyl group (H₃C) attached to the nitrogen atom. The stereochemistry is indicated with wedges and dashes. HBr HBr	EC number 411-000-9
129738-42-7	 The structure shows a cyclohexane derivative with a vinyl group (H₂C=CH-) attached to the ring. The stereochemistry is indicated with wedges and dashes.	 The structure shows a cyclohexane derivative with a vinyl group (H₂C=CH-) attached to the ring. The stereochemistry is indicated with wedges and dashes.	EC number 429-580-7

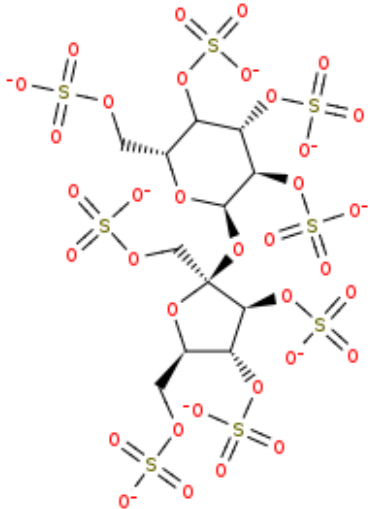
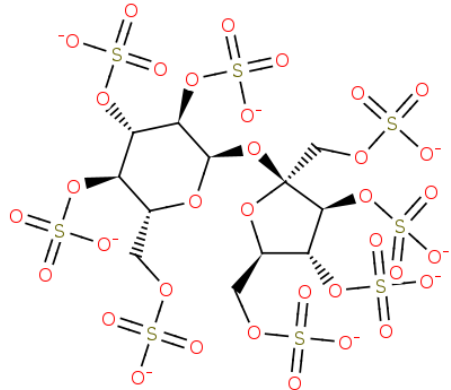
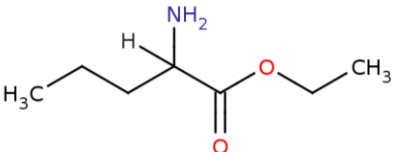
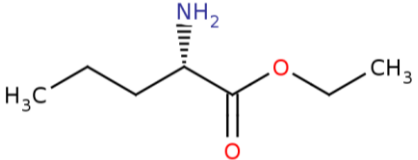
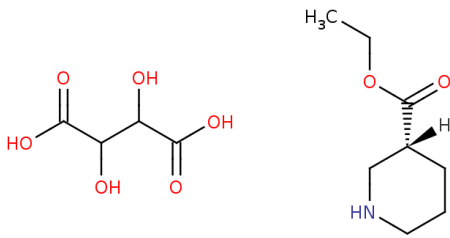
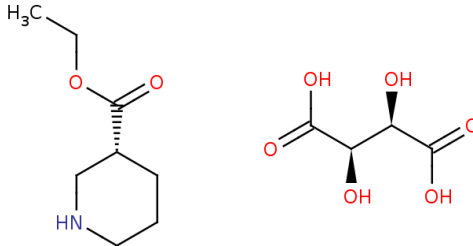
32981-86-5			EC number 418-680-6
31560-20-0			EC number 411-020-8
162537-11-3			EC number 431-620-3
478273-36-8			EC number 441-180-4

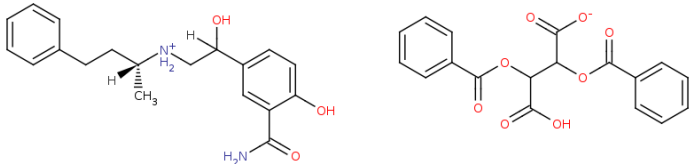
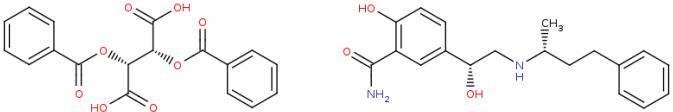
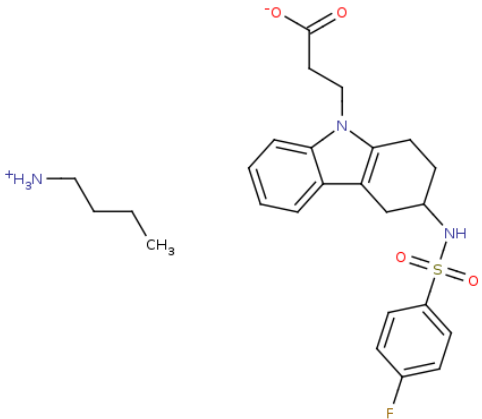
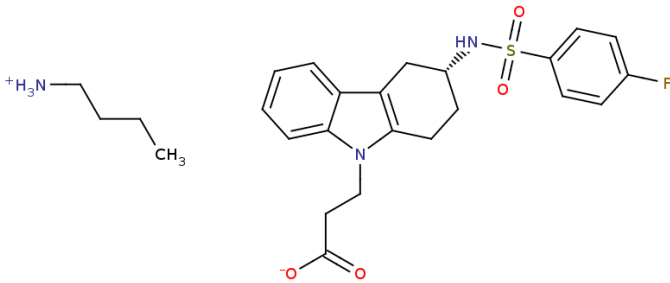
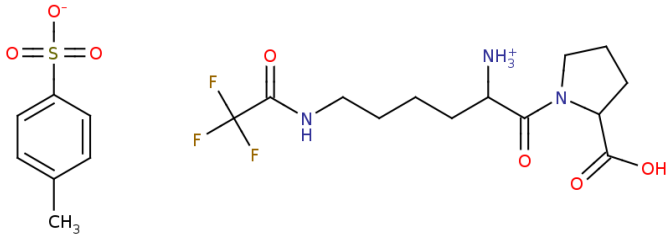
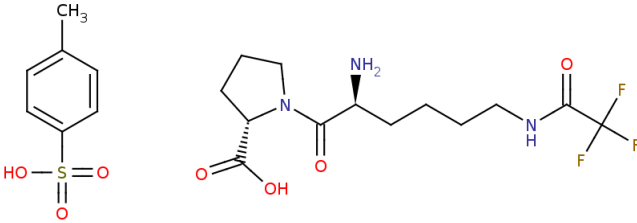
23477-67-0	 <chem>CC12CCC3C(C1)C(=O)CCC4C(C2)C(=O)C=C34</chem>	 <chem>CC12CCC3C(C1)C(=O)CCC4C(C2)C(=O)C=C34</chem>	EC number 419-120-3
124285-42-3	 <chem>CCCCCCCCCCCC(=O)OCC1OC(O)C(O)C(O)CO1</chem>	 <chem>CCCCCCCCCCCC(=O)OCC1OC(O)C(O)C(O)CO1</chem>	EC number 418-590-7
60166-91-8	 <chem>CC(=O)OC(C)C(=O)Nc1c(I)c(Cl)c(Cl)c1C(=O)Cl</chem>	 <chem>CC(=O)OC(C)C(=O)Nc1c(I)c(Cl)c(Cl)c1C(=O)Cl</chem>	EC number 410-940-7
103300-91-0	 <chem>CCCCNC(=O)C1CCCN1C(=O)C(Cc2ccccc2)C(=O)OCC</chem>	 <chem>CCCCNC(=O)C1CCCN1C(=O)C(Cc2ccccc2)C(=O)OCC</chem>	EC number 405-650-2

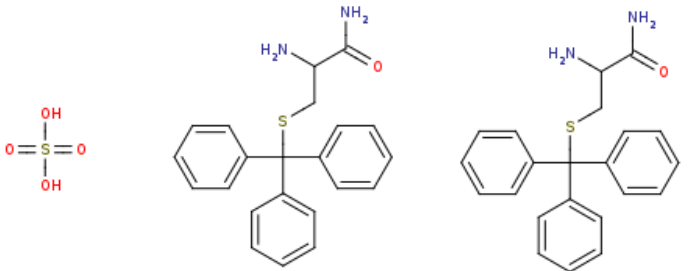
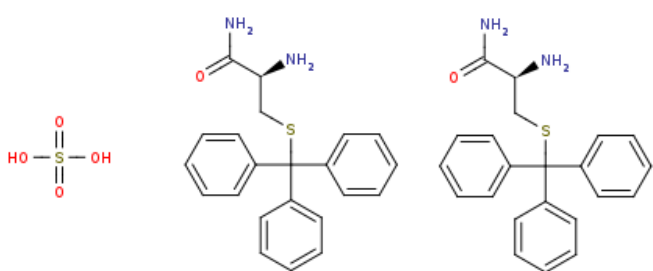
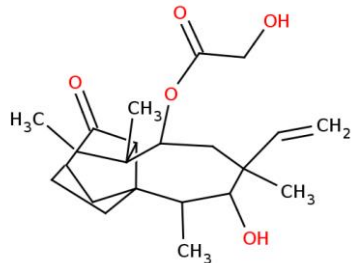
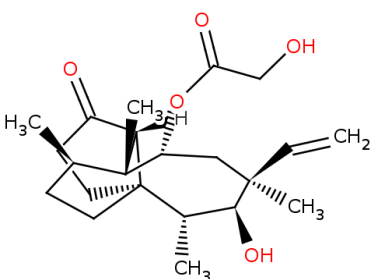
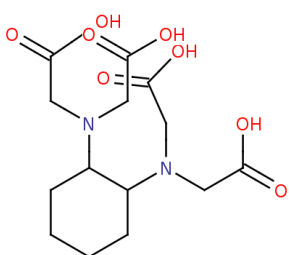
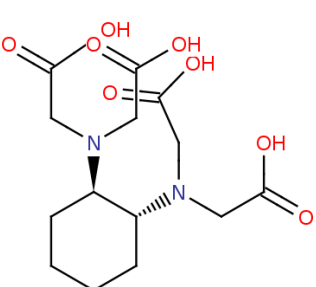
105351-42-6	 Chemical structure of 1,4-bis(4-prop-1-en-1-yl)cyclohexane, showing two cyclohexane rings connected at the 1 and 4 positions, with a prop-1-en-1-yl group attached to each ring.	 Chemical structure of 1,4-bis(4-prop-1-en-1-yl)-2,2'-bicyclohexyl, showing two cyclohexane rings connected at the 2 and 2' positions, with a prop-1-en-1-yl group attached to each ring at the 1 and 4 positions.	EC number 806-827-0
155522-12-6	 Chemical structure of 1-(4-chloro-2-nitrophenyl)-2-((4-((2-methoxy-1-oxoethyl)amino)phenyl)hydrazono)ethan-1-one, showing a benzene ring with a nitro group and a chlorine atom, connected via a hydrazone bridge to another benzene ring with an amino group and a methoxycarbonyl group.	 Chemical structure of 1-(4-chloro-2-nitrophenyl)-2-((4-((2-methoxy-1-oxoethyl)amino)phenyl)hydrazono)ethan-1-one, showing a benzene ring with a nitro group and a chlorine atom, connected via a hydrazone bridge to another benzene ring with an amino group and a methoxycarbonyl group.	EC number 416-240-8

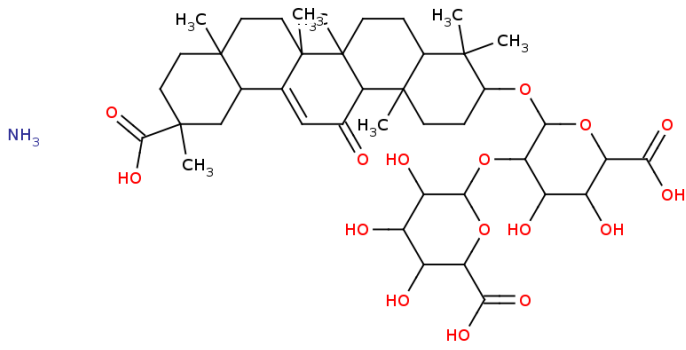
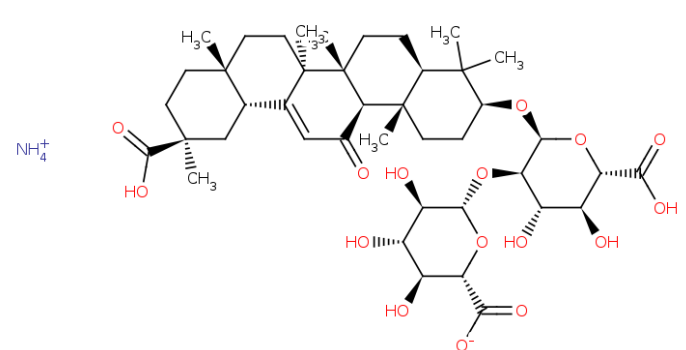
123560-48-5	 Chemical structure of 1-(2-ethoxy-3,4-difluorophenyl)-1,3-bis(cyclohexyl)propane. It features a central benzene ring substituted with two fluorine atoms (F) and an ethoxy group (OCH₂CH₃). This benzene ring is connected via a propyl chain to two cyclohexyl rings, which are further substituted with ethyl groups (CH₂CH₃).	 Chemical structure of 1-(2-ethoxy-3,4-difluorophenyl)-1,3-bis(cyclohexyl)propane. It features a central benzene ring substituted with two fluorine atoms (F) and an ethoxy group (OCH₂CH₃). This benzene ring is connected via a propyl chain to two cyclohexyl rings, which are further substituted with ethyl groups (CH₂CH₃).	EC number 602-941-8
49708-81-8	 Chemical structure of 4-chlorobenzylcyclohexanecarboxylic acid. It consists of a cyclohexane ring substituted with a carboxylic acid group (COOH) and a 4-chlorobenzyl group (CH₂-C₆H₄-Cl).	 Chemical structure of 4-chlorobenzylcyclohexanecarboxylic acid. It consists of a cyclohexane ring substituted with a carboxylic acid group (COOH) and a 4-chlorobenzyl group (CH₂-C₆H₄-Cl).	EC number 406-380-8

926276-18-8			EC number 482-250-4
6863-90-7			EC number 417-860-1

74135-10-7	 Na⁺ Na⁺ Na⁺ Na⁺ Na⁺ Na⁺ Na⁺ Na⁺	 Na⁺ Na⁺ Na⁺ Na⁺ Na⁺ Na⁺ Na⁺ Na⁺	EC number 420-660-7
40918-51-2	HCl 	 HCl	EC number 482-890-4
83602-37-3			EC number 421-850-2

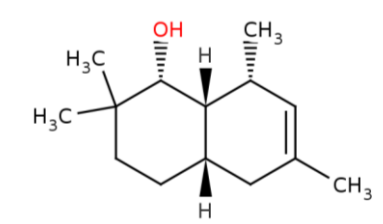
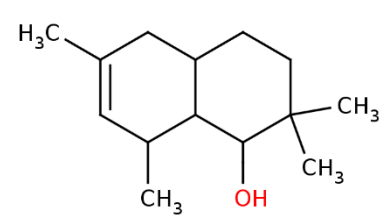
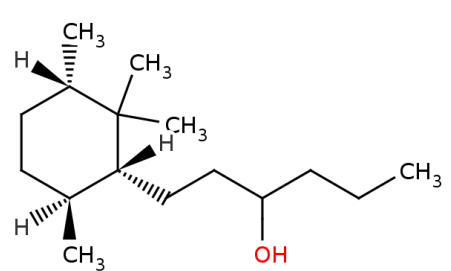
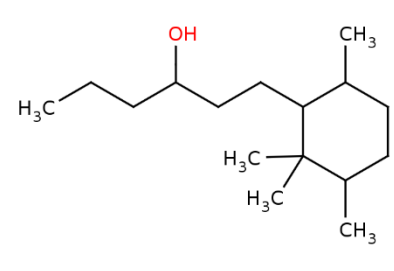
88976-55-0			EC number 404-390-7
1182723-73-4			EC number 925-462-9
105641-23-4			EC number 402-160-0

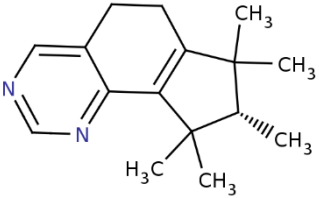
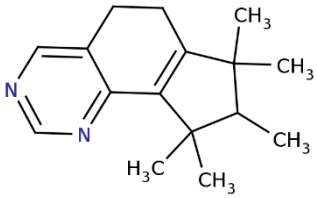
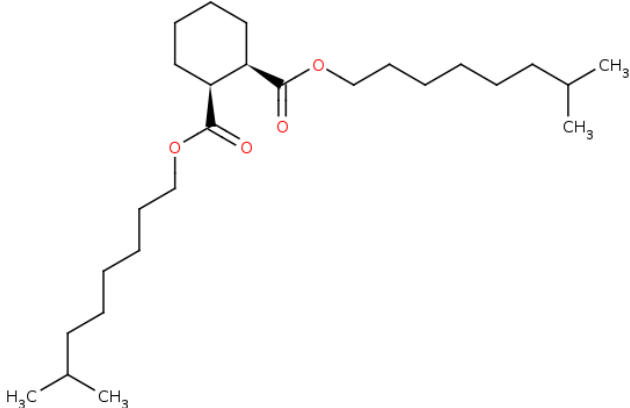
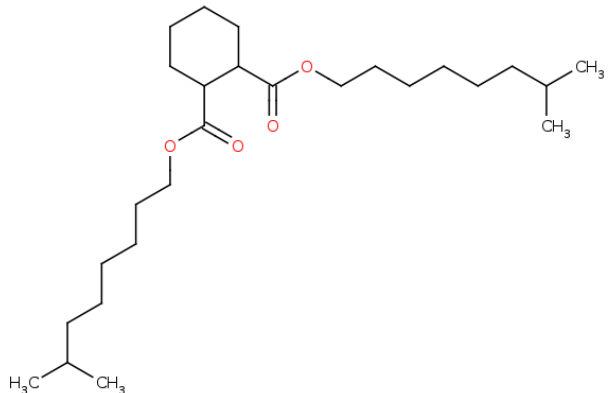
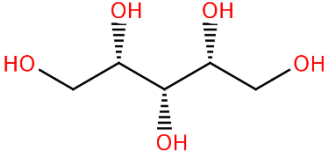
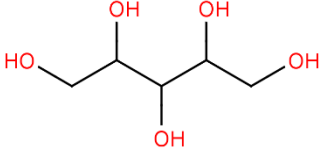
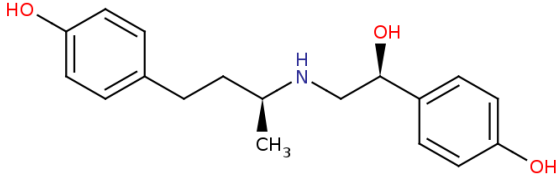
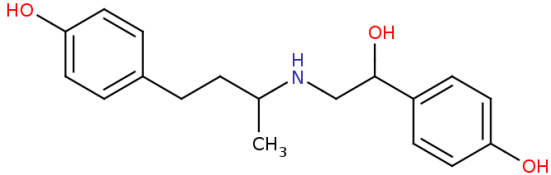
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125-65-5			EC number 204-747-5
13291-61-7			EC number 236-308-9

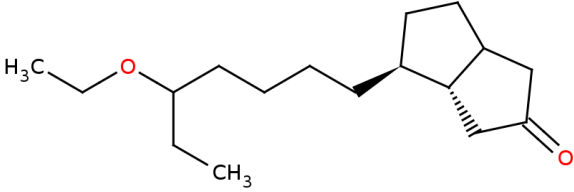
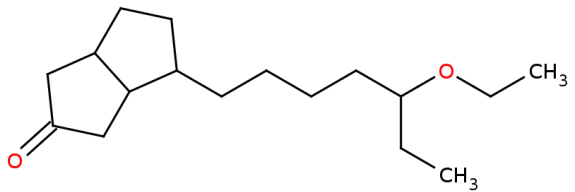
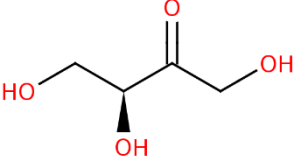
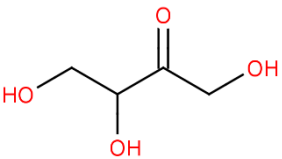
53956-04-0			EC number 258-887-7
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7) Inconsistencies related to the stereochemistry (available stereochemistry information in the ECHA database were SciFinderⁿ has none)

Table 7: Substances in the ECHA database where the SMILES do not correspond to the CAS RNTM as allocated in SciFinderⁿ. The reason for the mismatches here are available stereochemistry information in the ECHA database were SciFinderⁿ has none.

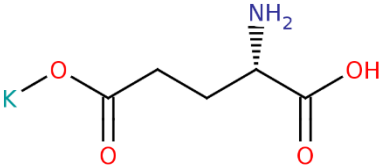
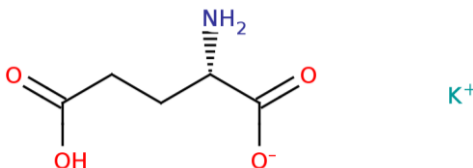
CAS RN TM	Structure in the database	Structure corresponding to the CAS RN TM	Comment
103614-86-4			EC number 434-960-0
95851-08-4			EC number 478-330-3

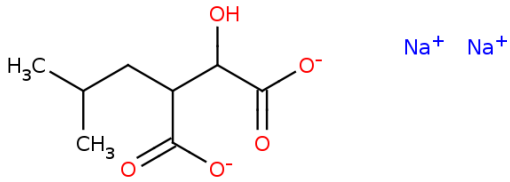
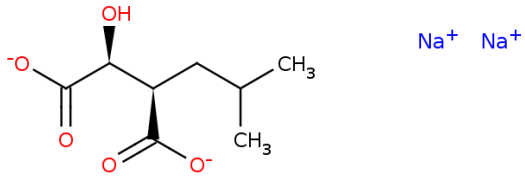
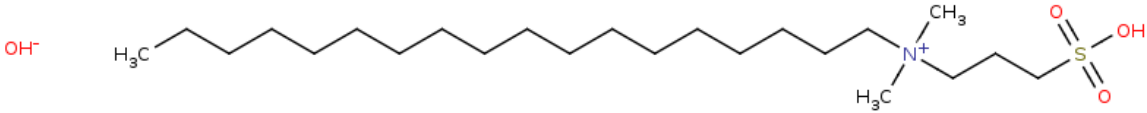
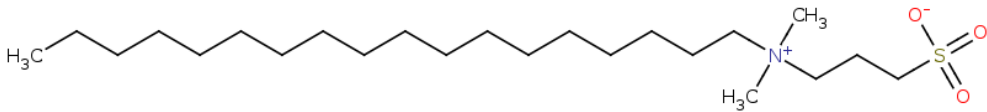
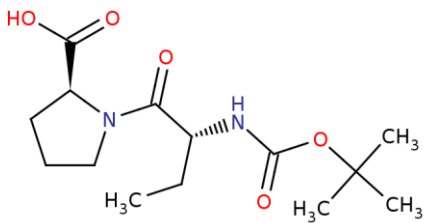
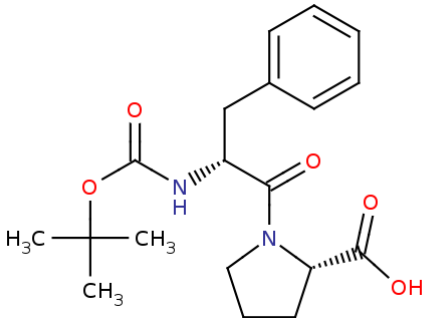
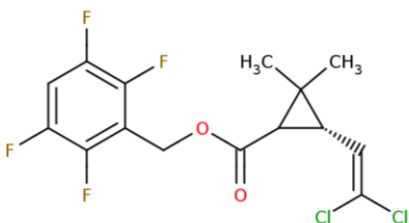
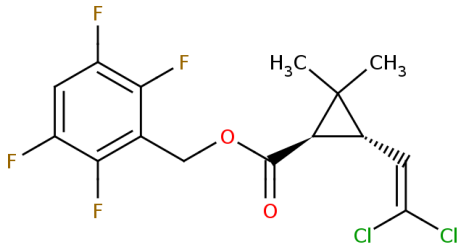
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166412-78-8			EC number 431-890-2
87-99-0			EC number 201-788-0
90274-24-1	HCl 	HCl 	EC number 415-170-5

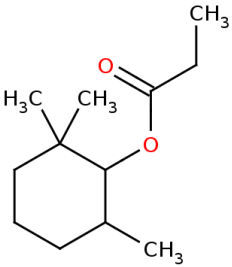
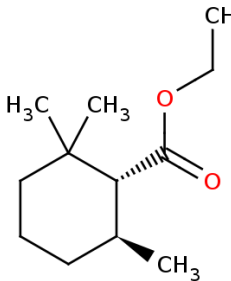
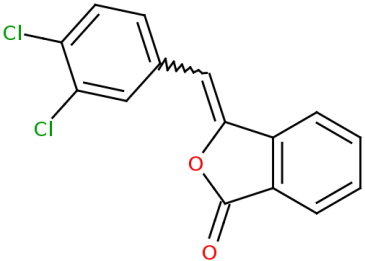
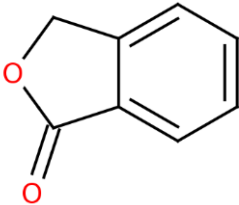
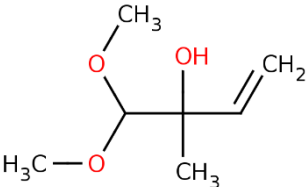
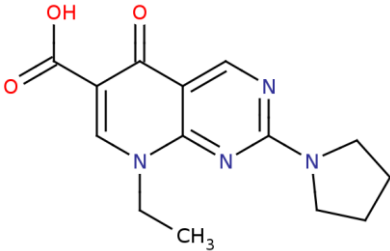
106-89-8			EC number 482-080-0
99778-68-4			EC number 419-880-6
40031-31-0			EC number 443-800-9

8) Substances not included in this study that were assessed after the submission

Table 8: Substances in the ECHA database that are not included in this study but were assessed after the submission

CAS RN™	Structure in the database	Structure corresponding to the CAS RN™	Comment
19473-49-5			EC number 243-094-0

2136268-40-9			EC number 428-800-9
13177-41-8 (in consistent form)			EC number 236-124-9
13177-41-8 (consistent form)			EC number 236-124-9
38675-10-4			EC number 448-070-5
118712-89-3			EC number 405-060-5

22471-55-2	 Chemical structure of 2-ethoxy-2,2-dimethyl-4-methylcyclohexan-1-ol. It features a cyclohexane ring with an ethoxy group (-OCH₂CH₃) and two methyl groups on one carbon, and another methyl group on the carbon at the 4-position.	 Chemical structure of 2-ethoxy-2,2-dimethyl-4-methylcyclohexan-1-ol, showing stereochemistry with a wedged methyl group at the 4-position and a dashed ethoxy group at the 1-position.	EC number 412-540-8
87-41-2	 Chemical structure of 2-(2,4-dichlorophenyl)-2,3-dihydro-1H-benzofuran-3-one. It consists of a benzofuranone core with a 2,4-dichlorophenyl group attached at the 2-position.	 Chemical structure of 1-benzobicyclo[3.2.1]oct-2-ene-3-one. It features a benzene ring fused to a bicyclic system containing an enone moiety.	EC number 417-930-1
19562-30-2	 Chemical structure of 2-ethoxy-2-methyl-3-methoxy-3-methylbut-3-en-2-ol. It is a branched molecule with a central carbon atom bonded to a hydroxyl group, a methyl group, a methoxy group, and a 2-ethoxy-2-methylbut-3-en-2-yl group.	 Chemical structure of 1-ethyl-6-(cyclopentylamino)pyrimidin-2(1H)-one. It features a pyrimidin-2(1H)-one core with an ethyl group at the 1-position and a cyclopentylamino group at the 6-position.	EC number 419-730-1