Electronic Supplementary Material (ESI) for Environmental Science: Advances.

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

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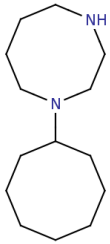
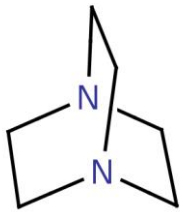
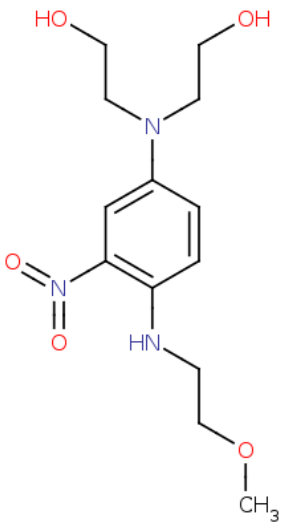
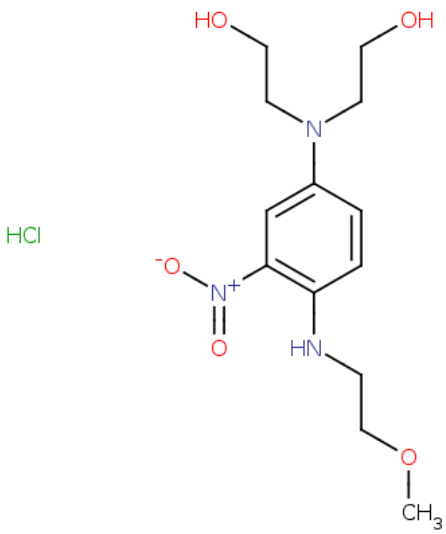
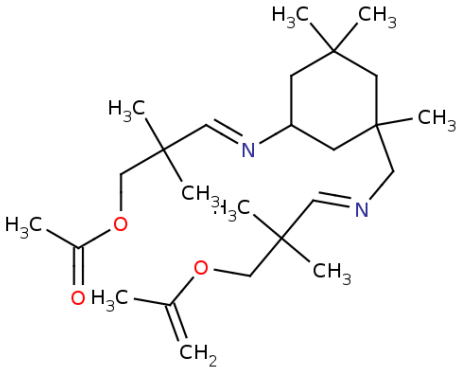
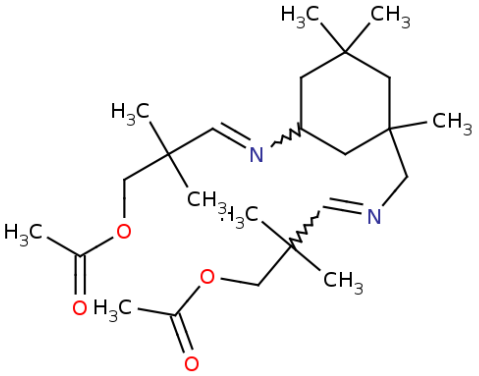
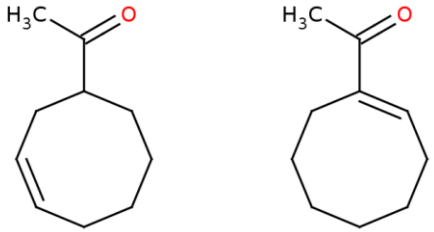
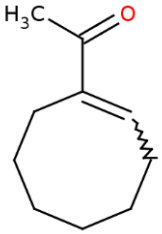
Substances in the ECHA database where the SMILES do not correspond to the Chemical Abstract Service Registry Number™ (CAS RN™) as allocated in SciFinder^{n}

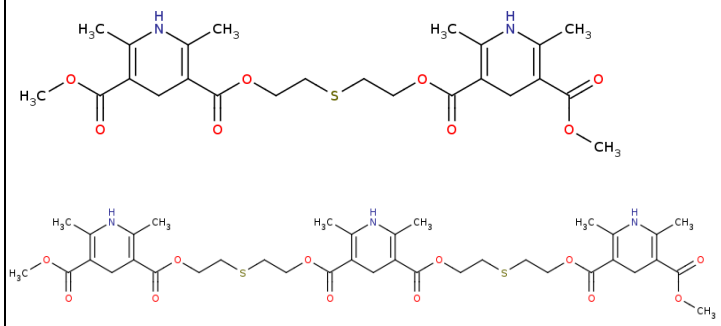
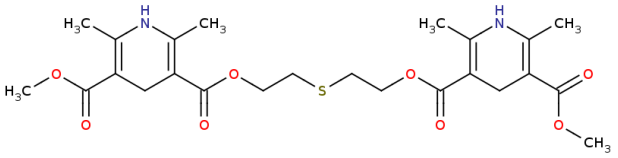
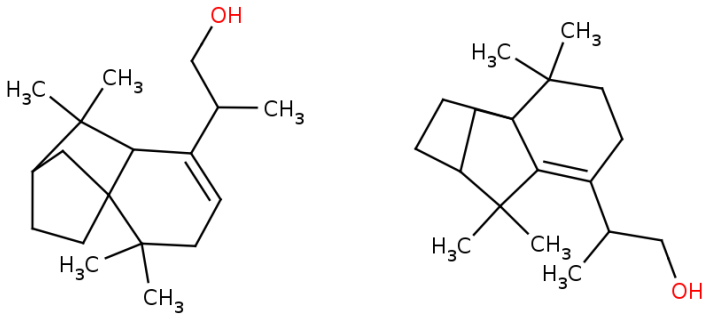
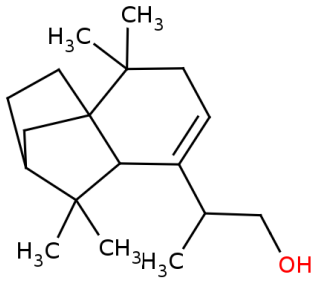
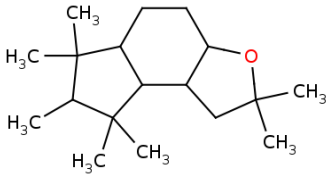
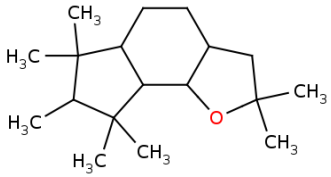
For the SMILES and names of the compounds, please refer to the Supporting Information-1 of this article. Please note that due to the large number of structures, mistakes cannot be excluded completely, and we assume no liability for the molecules shown. The information shown here correspond to the ECHA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

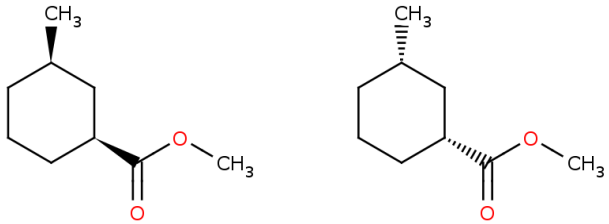
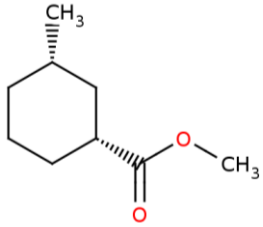
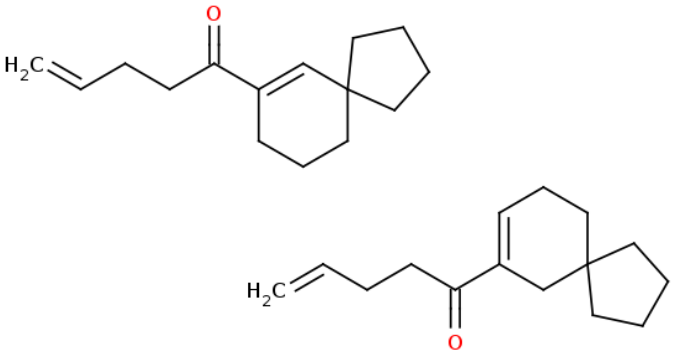
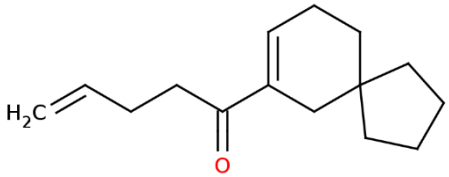
1) Inconsistency related to the molecular structure itself

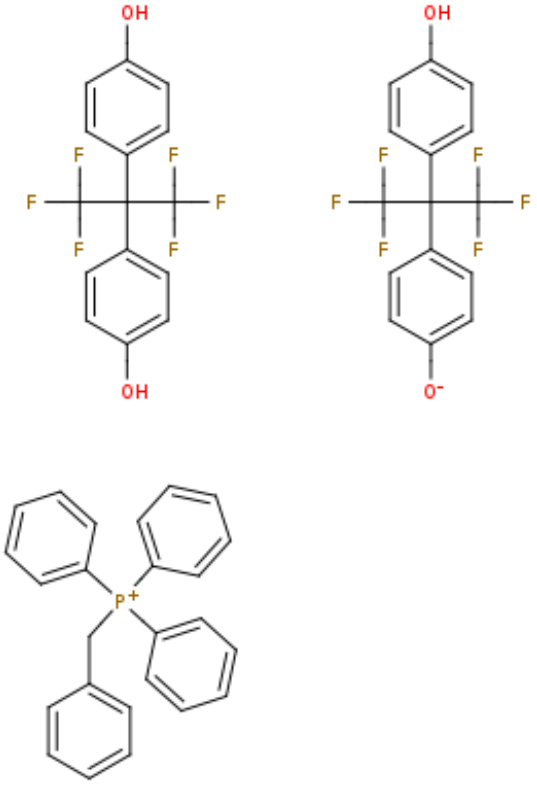
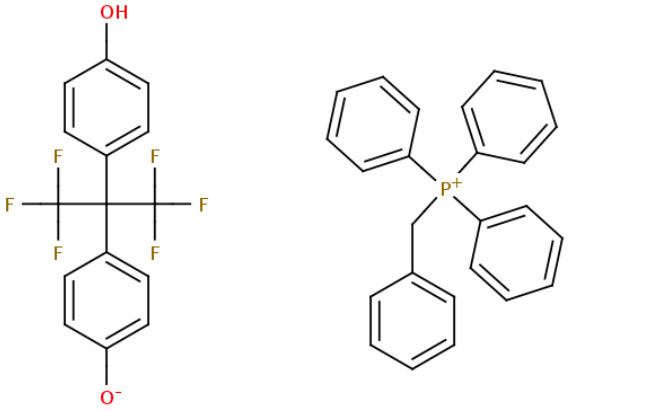
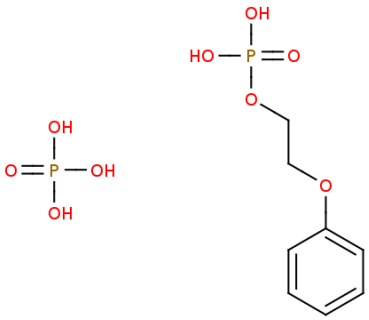
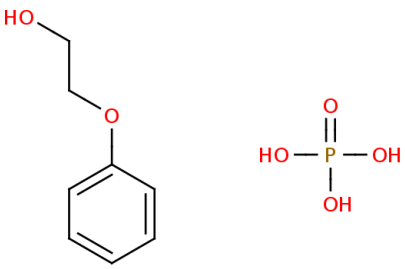
Table 1: Substances in the ECHA database where the SMILES do not correspond to the Chemical Abstract Service Registry Number™ (CAS RN™) as allocated in SciFinder^{n}. The reason for the mismatch is here the structures itself.

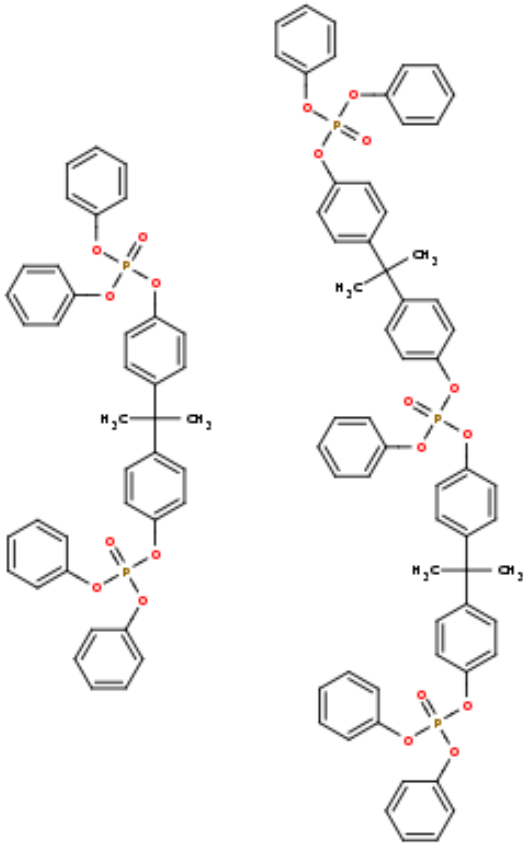
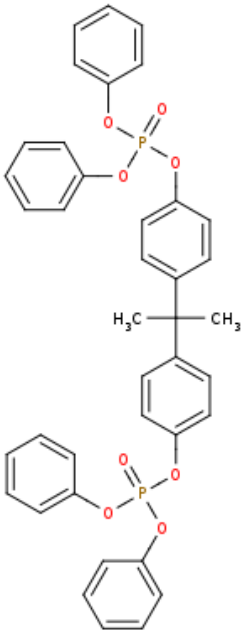
CAS RN™	Structure in the database	Structure corresponding to the CAS RN™	Comment
280-57-9			EC number 205-999-9

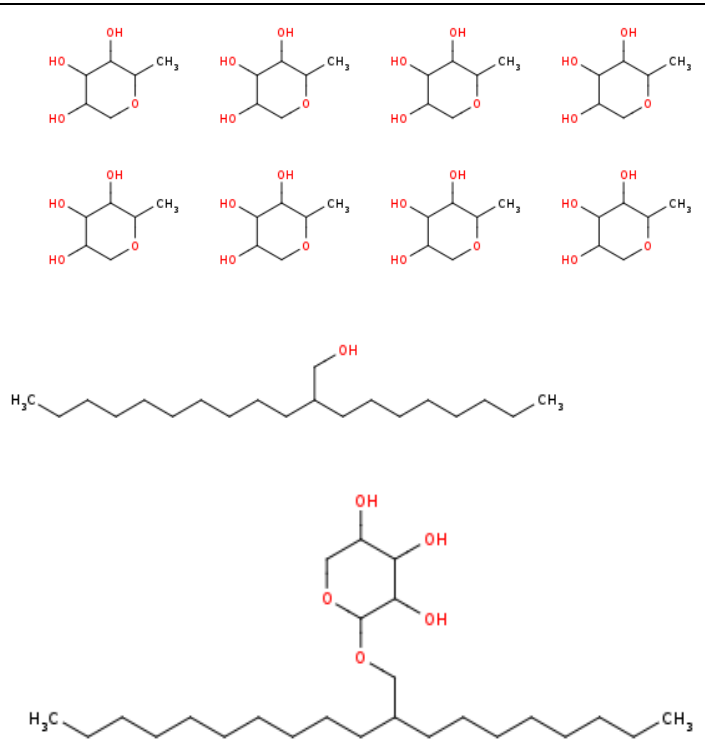
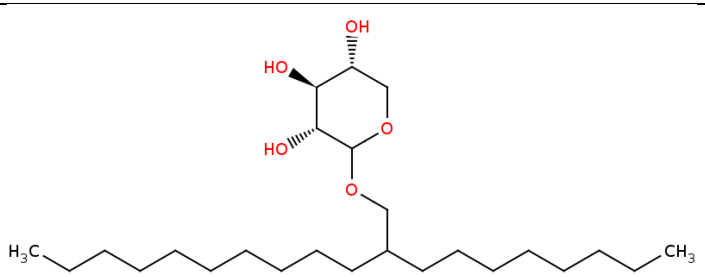
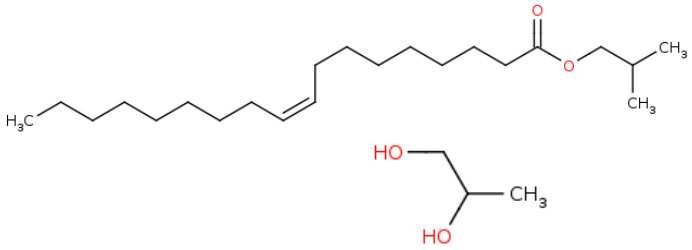
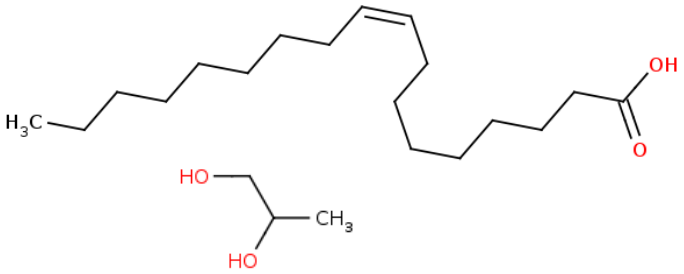
910463-51-3			EC number 459-980-7
1064082-81-0			EC number 805-722-7
17339-74-1			EC number 466-270-0 “correct” structure has still missing stereoinformation

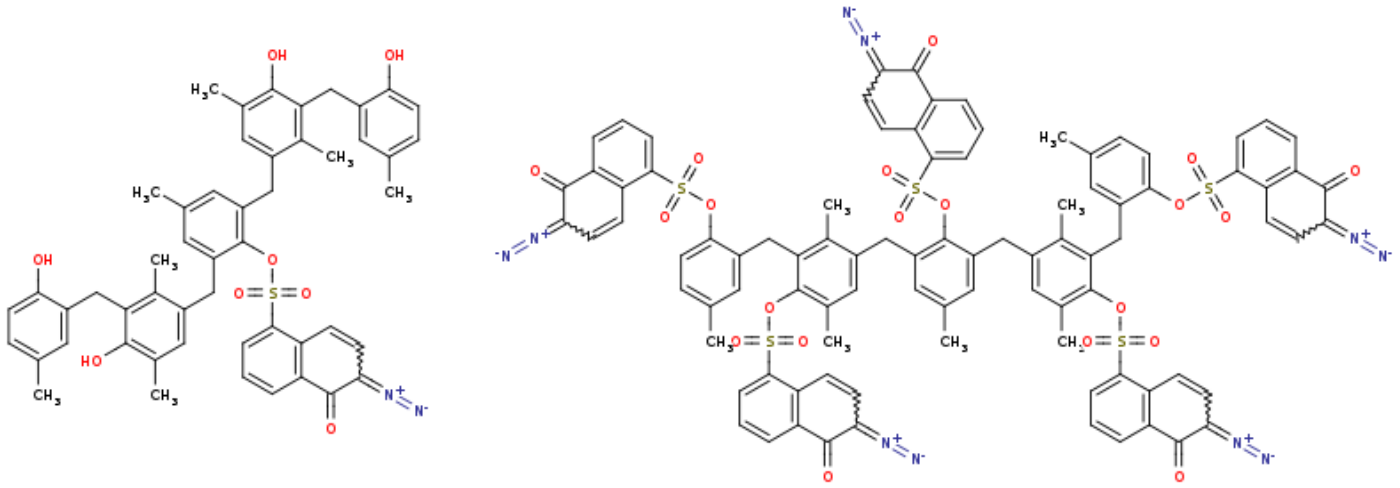
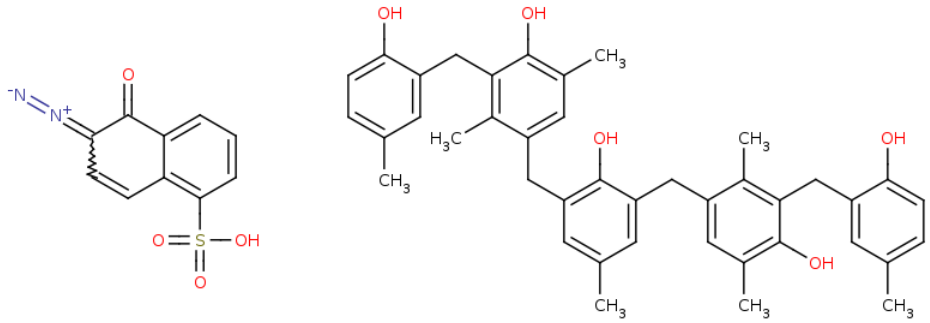
120218-34-0			EC number 404-440-8
1001252-30-7			EC number 482-030-8
647828-16-8			EC number 449-360-4

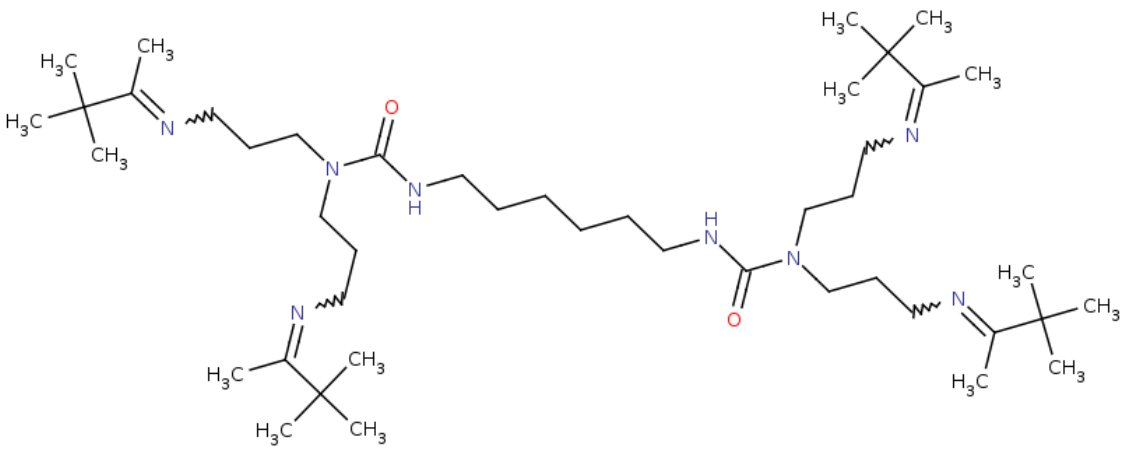
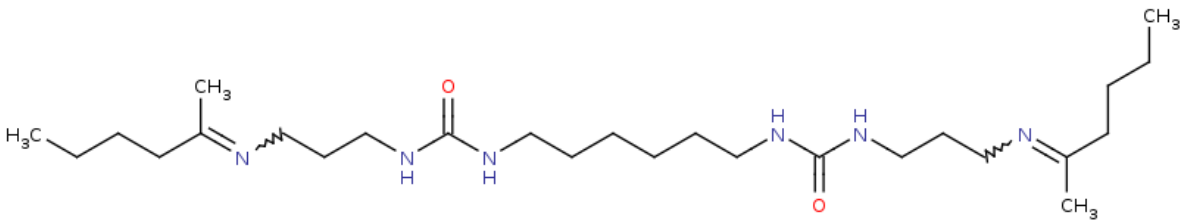
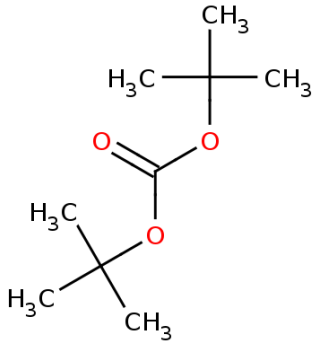
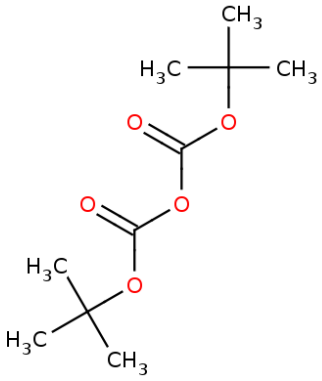
7605-52-9			EC number 700-420-0
224031-70-3			EC number 438-060-9

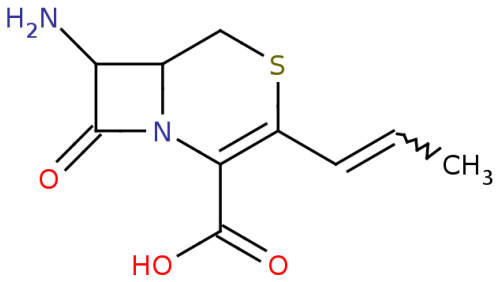
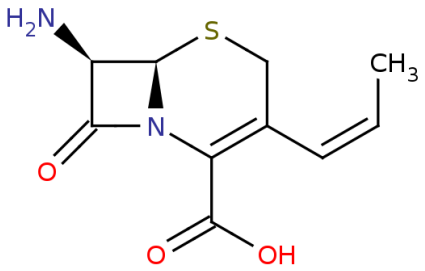
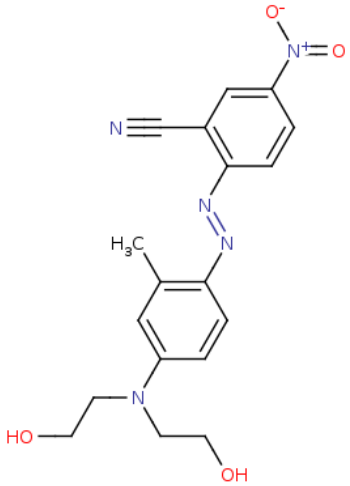
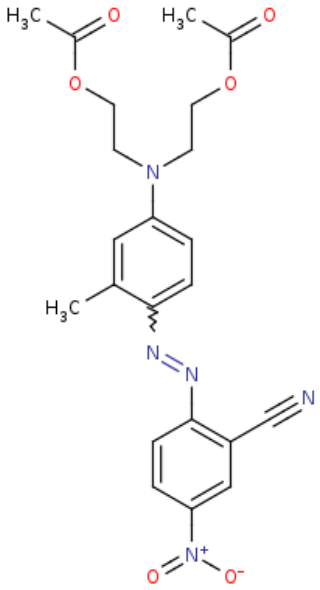
75768-65-9			EC number 278-305-5
39464-70-5			EC number 609-691-9

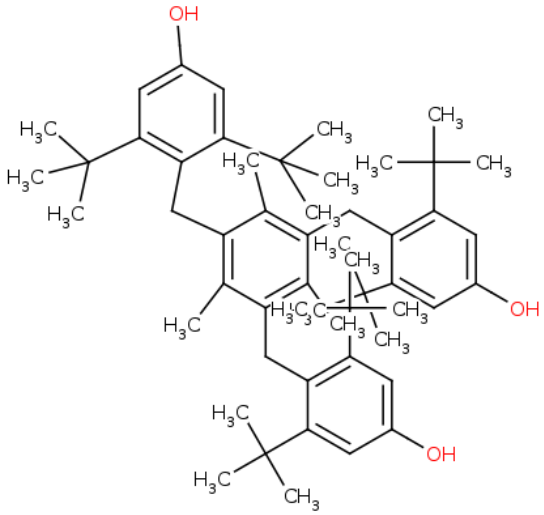
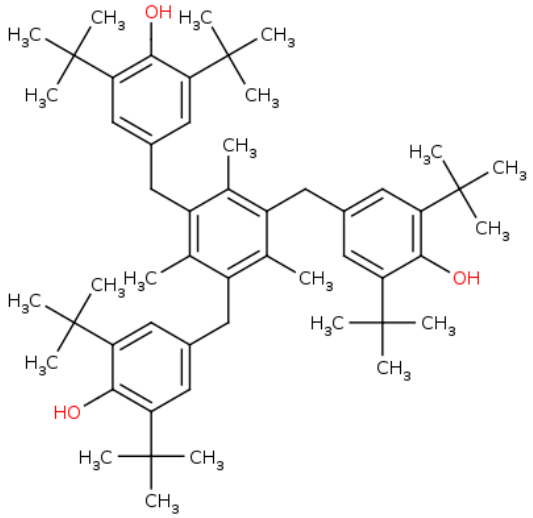
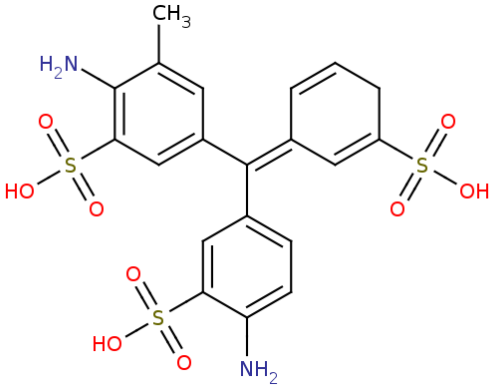
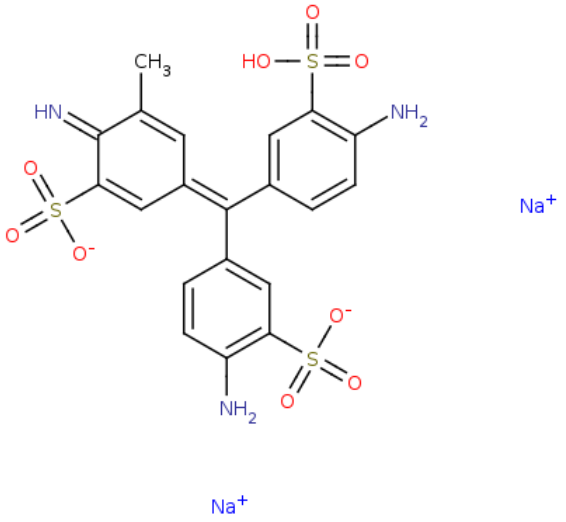
5945-33-5			EC number 425-220-8

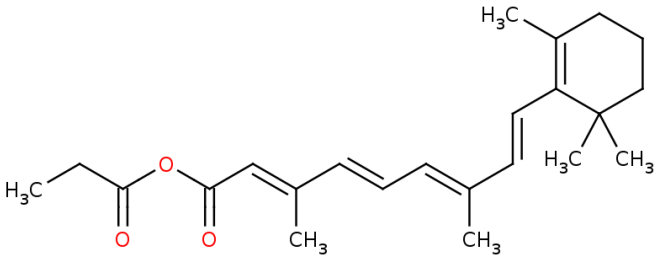
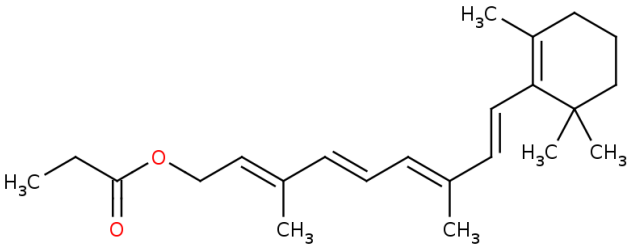
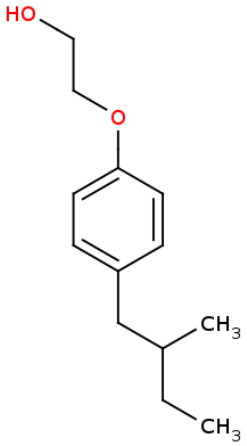
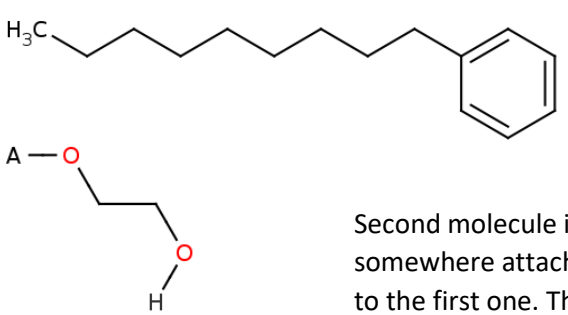
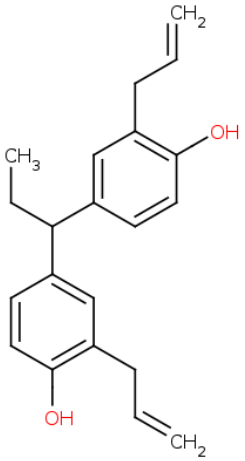
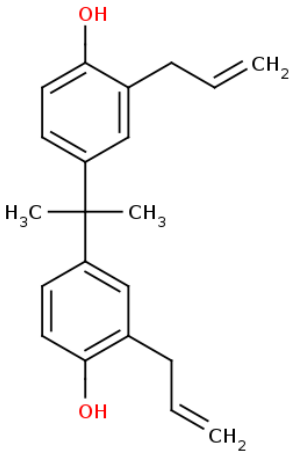
423772-95-6			EC number 464-320-6
1330-80-9			EC number 215-549-3

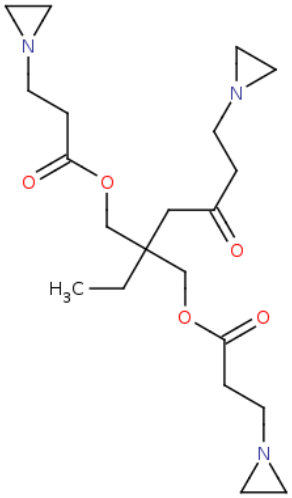
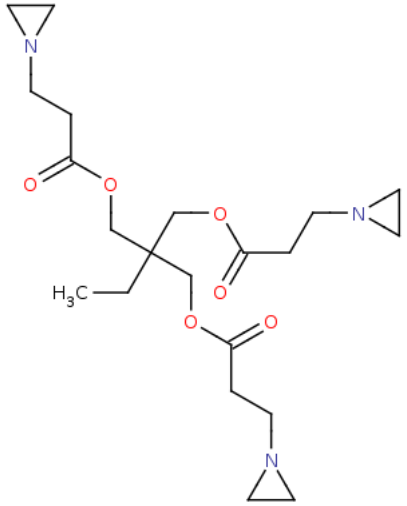
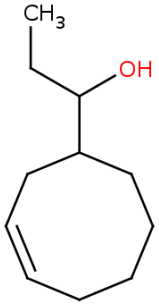
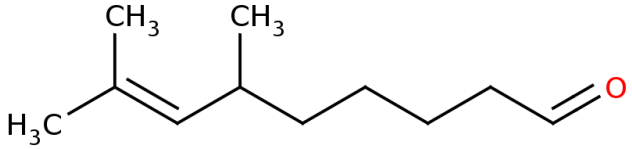
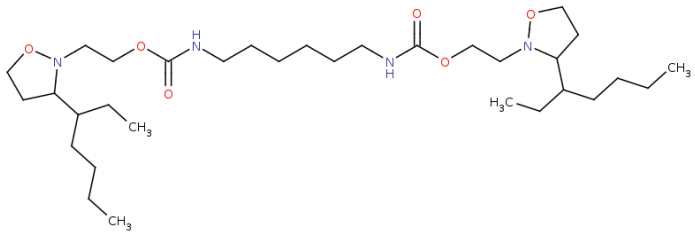
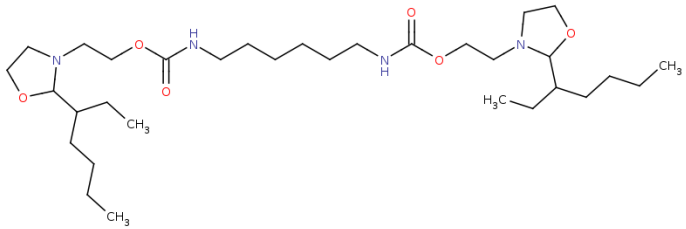
190394-85-5 (incorrect)		EC number 466-400-6
190394-85-5 (correct)		EC number 466-400-6

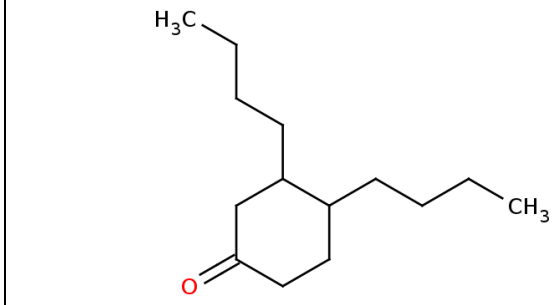
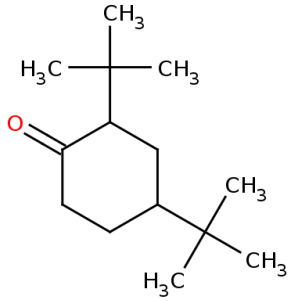
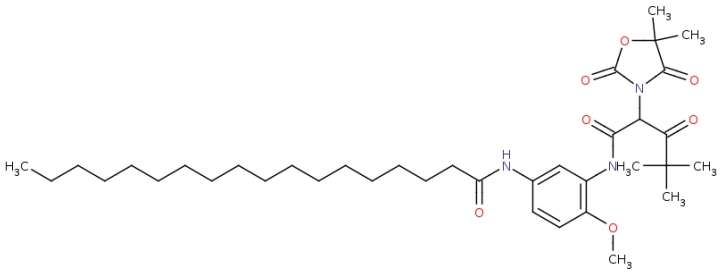
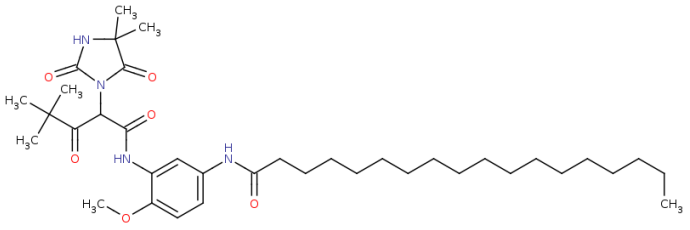
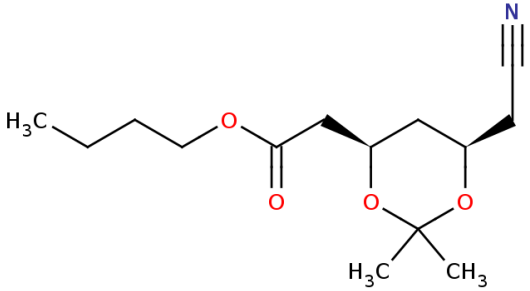
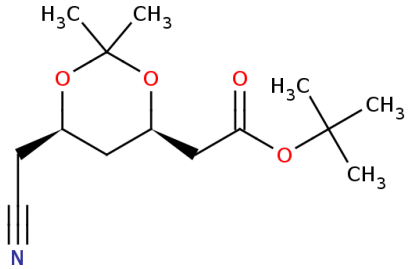
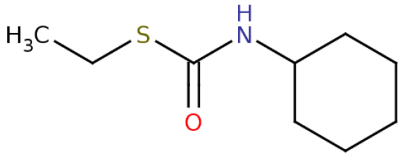
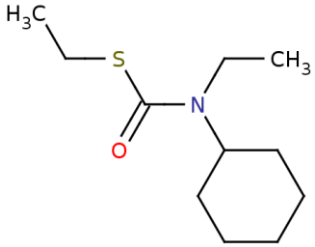
771478-66-1 (incorrect)		EC number 420-190-2
771478-66-1 (correct)		EC number 420-190-2
24424-99-5	 	EC number 246-240-1

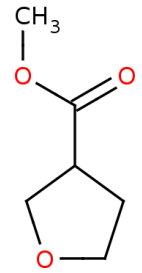
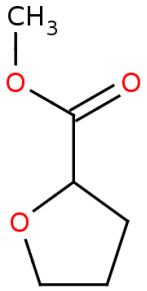
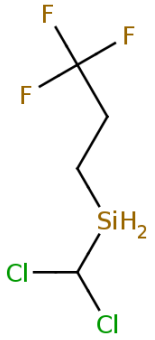
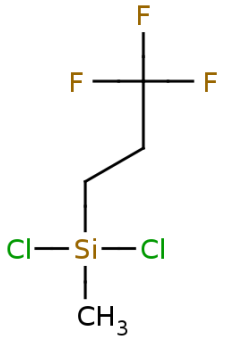
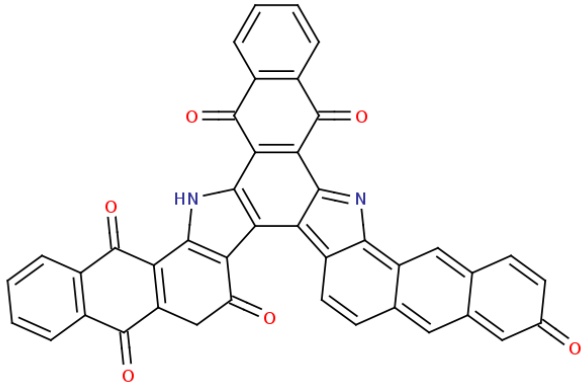
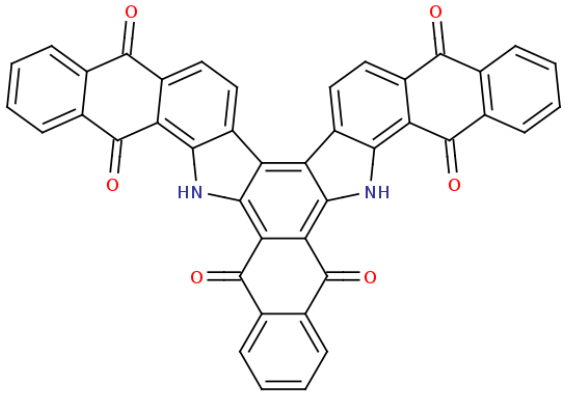
106447-44-3			EC number 415-750-8
12236-25-8			EC number 235-460-3

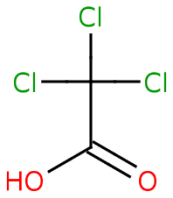
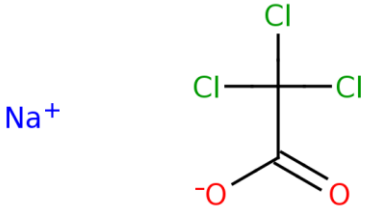
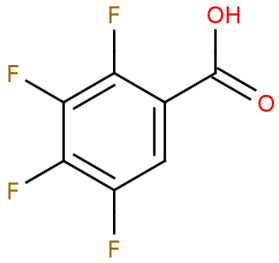
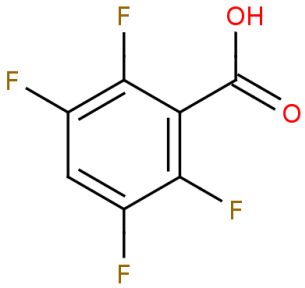
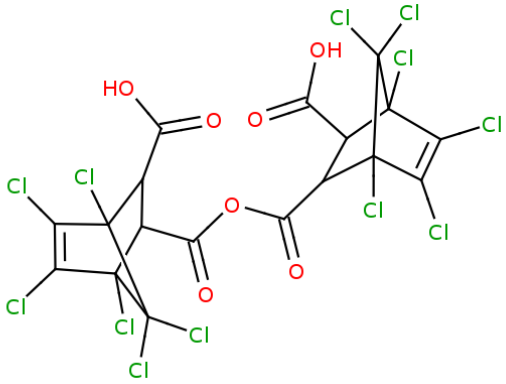
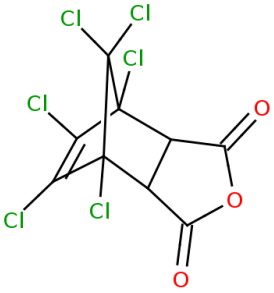
1709-70-2			EC number 216-971-0
3244-88-0			EC number 221-816-5

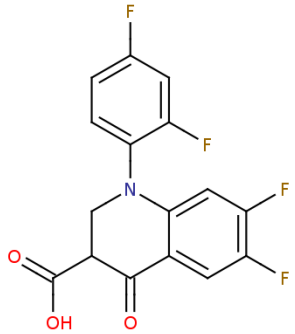
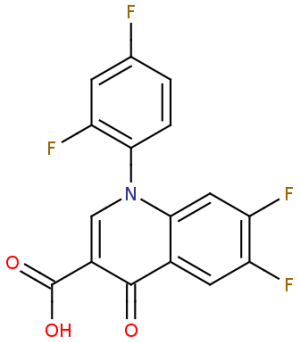
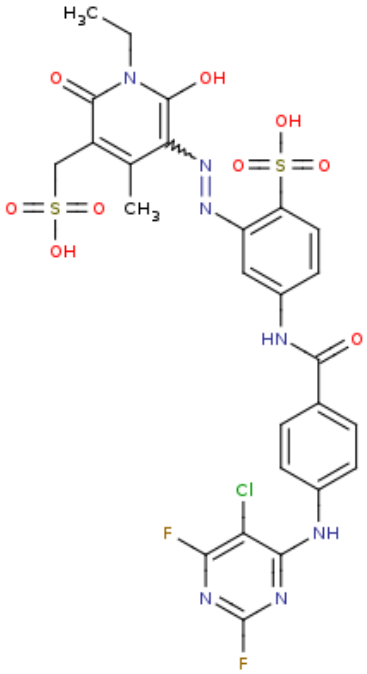
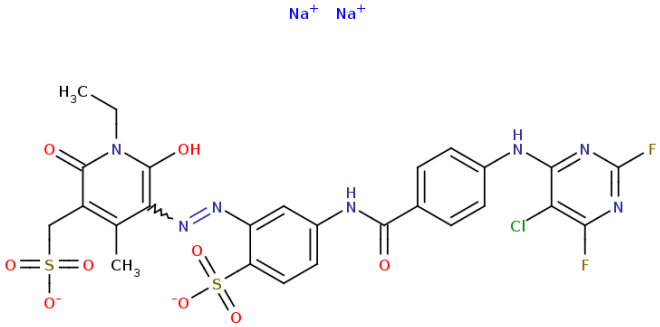
7069-42-3			EC number 230-363-2
9016-45-9		CAS RN represents polymer with the monomer units shown here  Second molecule is somewhere attached to the first one. The attachment point is 'A'	EC number 500-024-6
1745-89-7			EC number 217-121-1

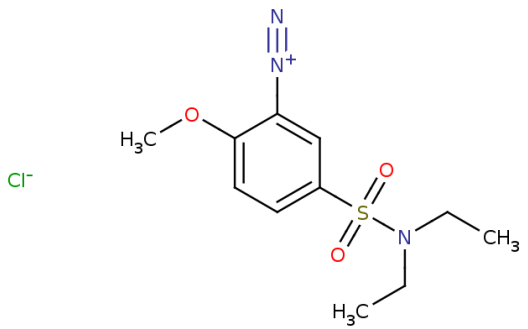
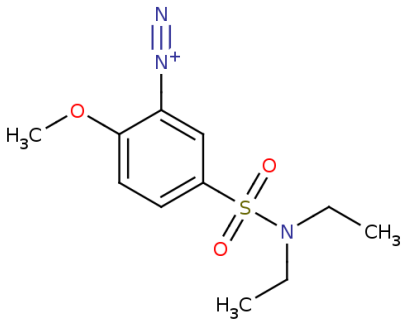
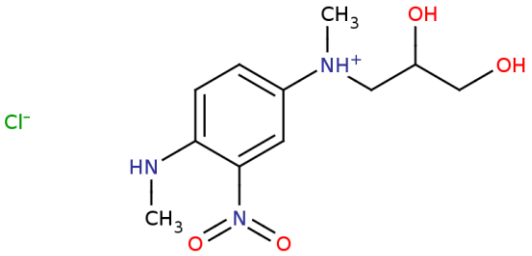
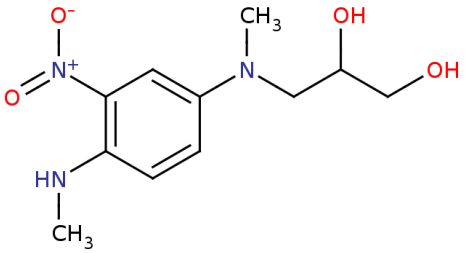
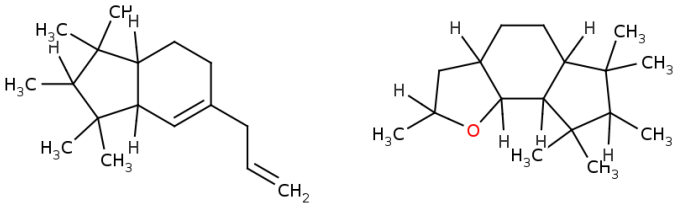
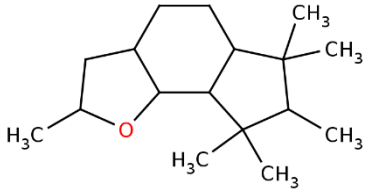
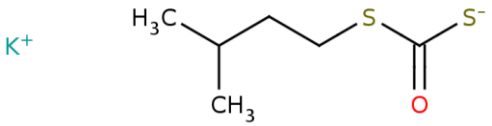
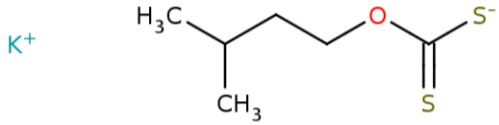
52234-82-9			EC number 257-765-0
899810-84-5			EC number 476-140-5
140921-24-0			EC number 411-700-4

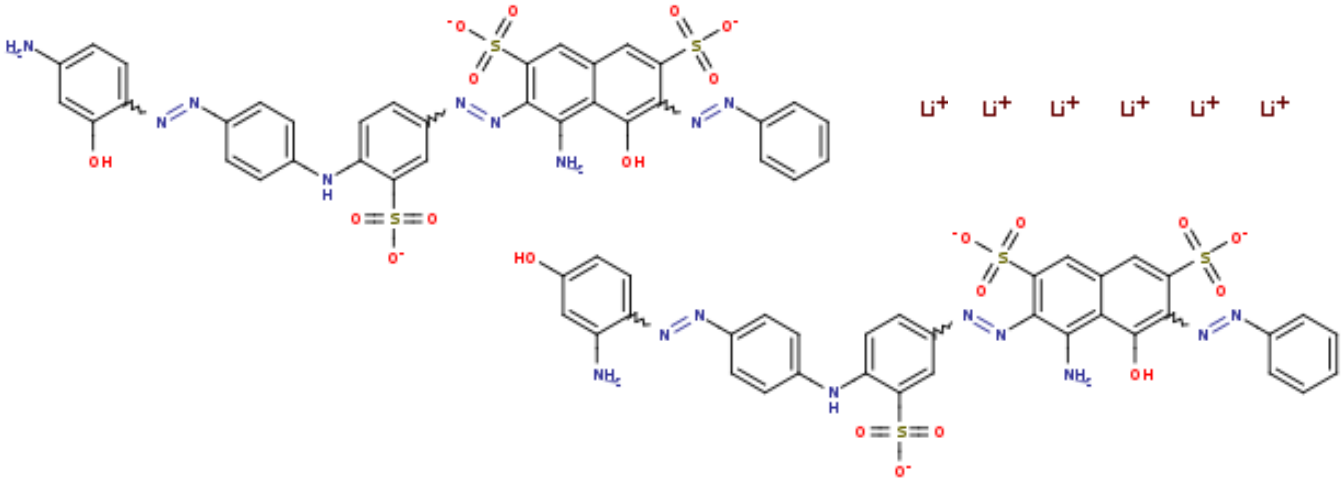
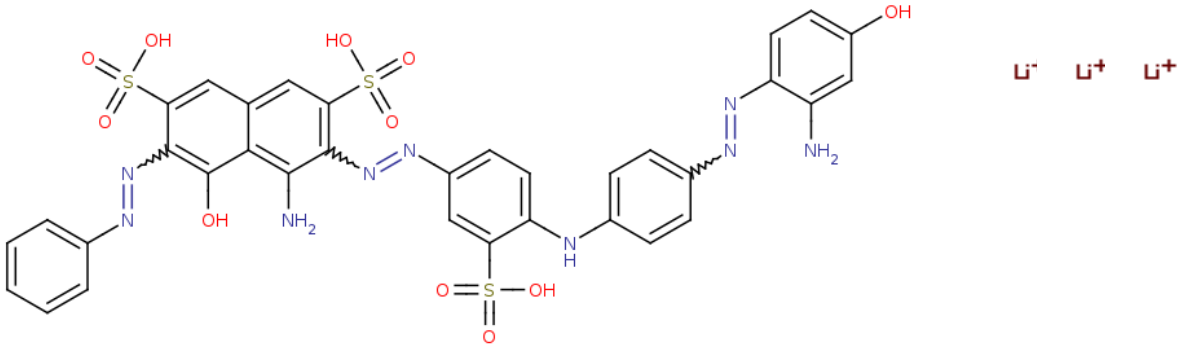
13019-04-0			EC number 405-340-7
221215-20-9			EC number 443-980-9
125971-94-0			EC number 425-780-3
1134-23-2			EC number 214-482-7

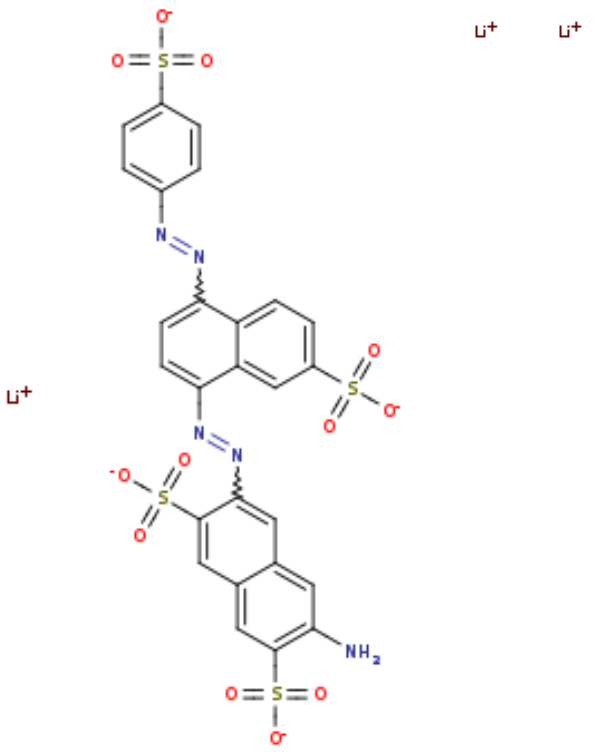
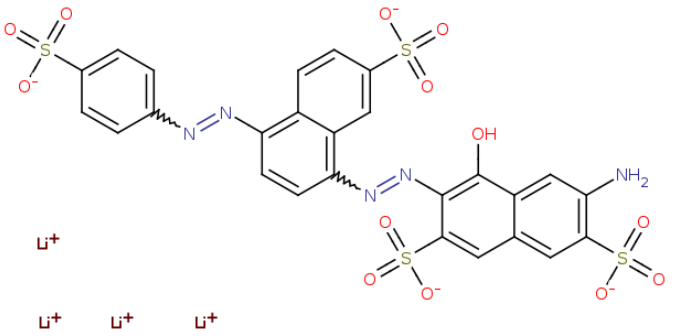
37443-42-8			EC number 420-670-1
675-62-7			EC number 211-623-4
2475-33-4			EC number 219-599-7

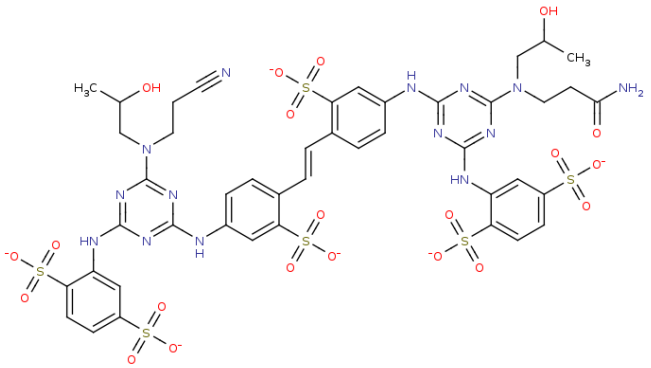
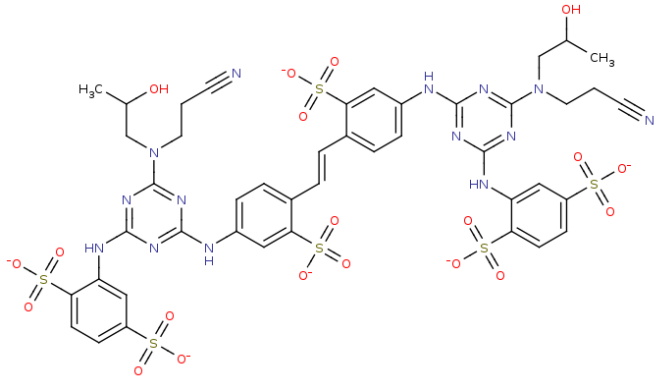
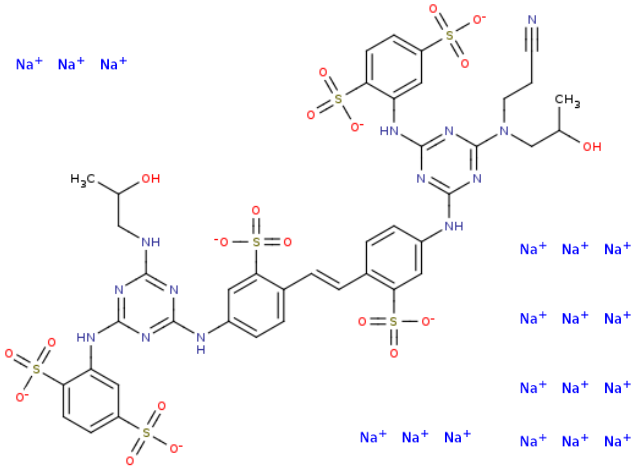
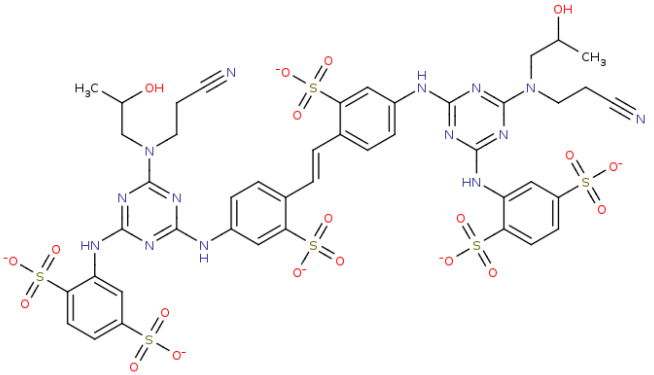
650-51-1			EC number 211-479-2
652-18-6			EC number 435-890-3
115-27-5			EC number 204-077-3

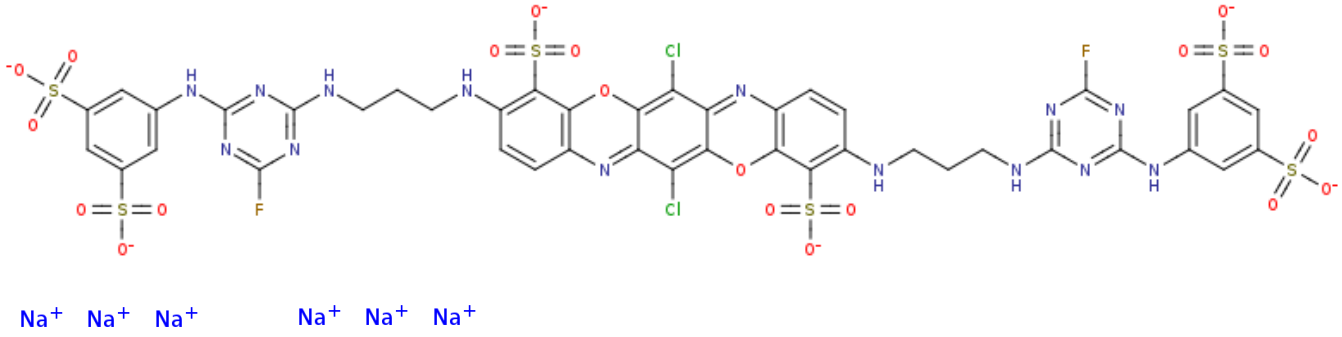
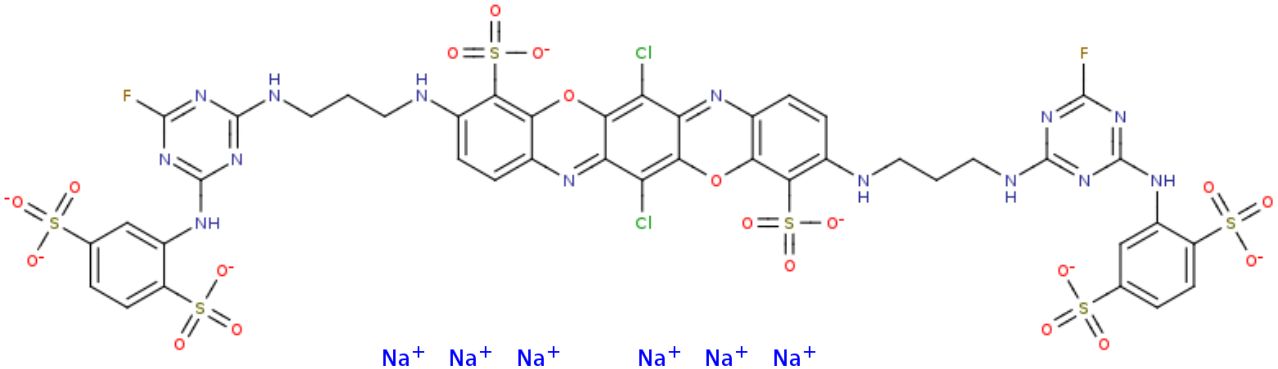
103995-01-3			EC number 406-710-0
157627-98-0			EC number 412-530-3

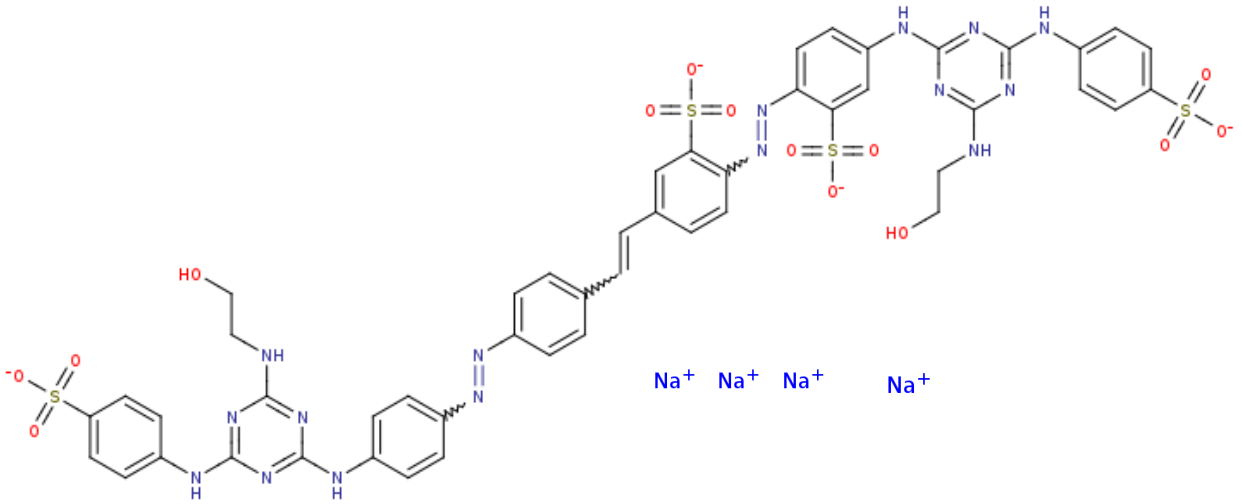
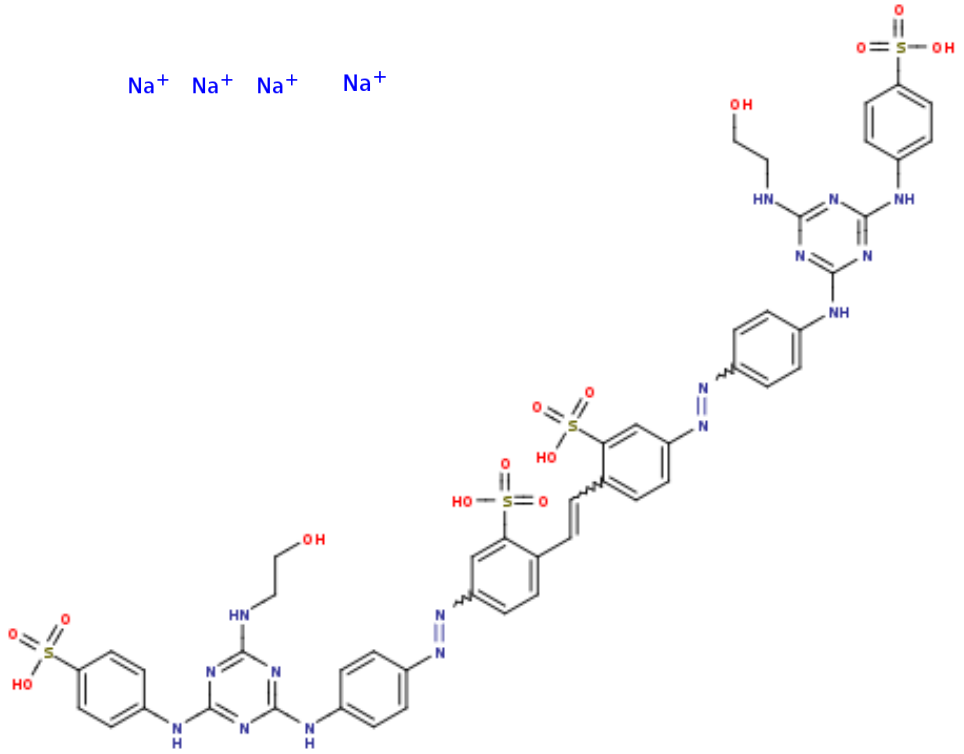
27580-14-9			EC number 248-543-4
93633-79-5			EC number 403-440-5
338735-71-0			EC number 440-030-5
928-70-1			EC number 213-180-2

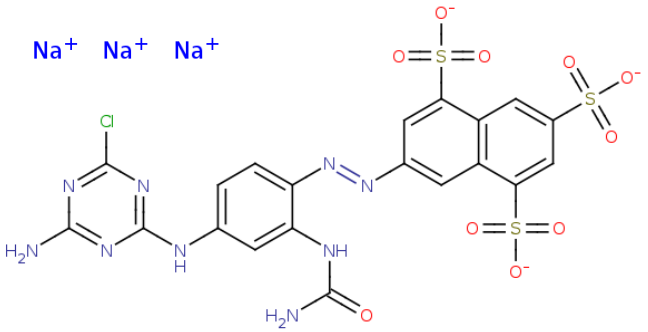
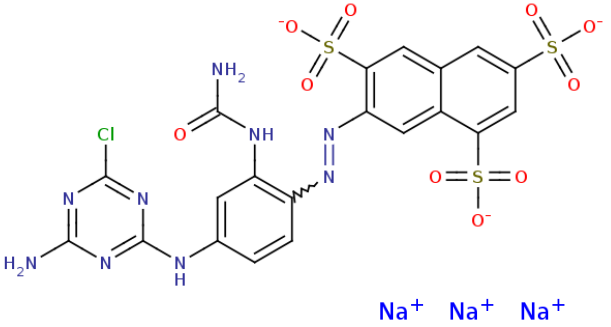
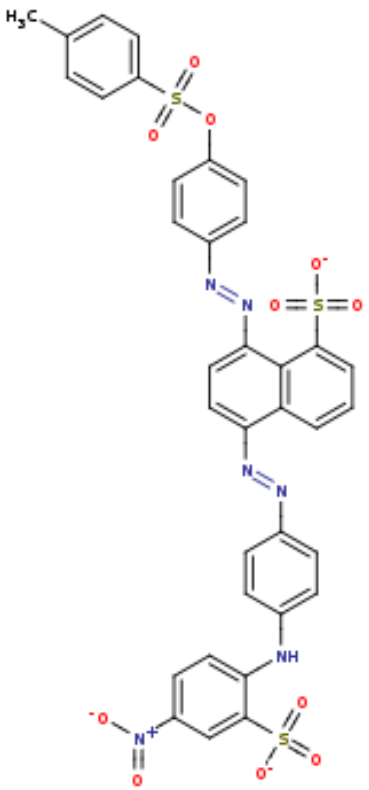
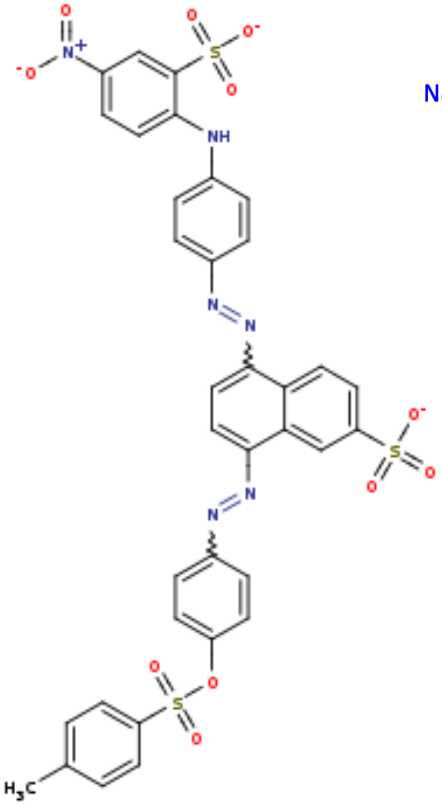
108936-08-9 (incorrect form)		EC number 411-890-9
108936-08-9 (correct form)		EC number 411-890-9 CAS RN™ includes only the second structure

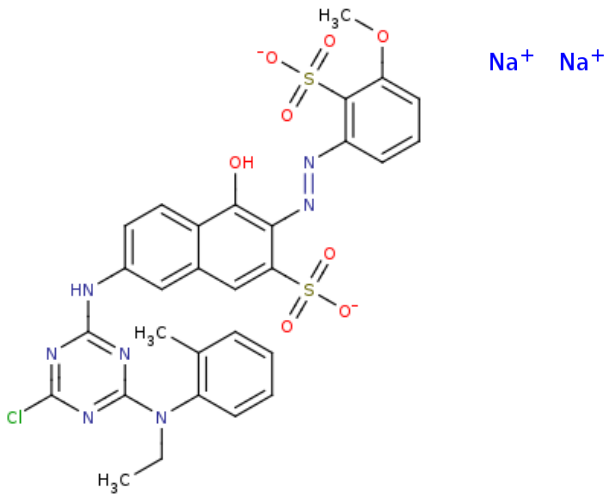
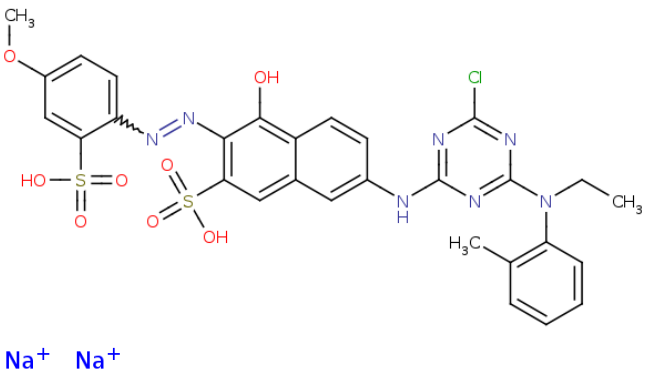
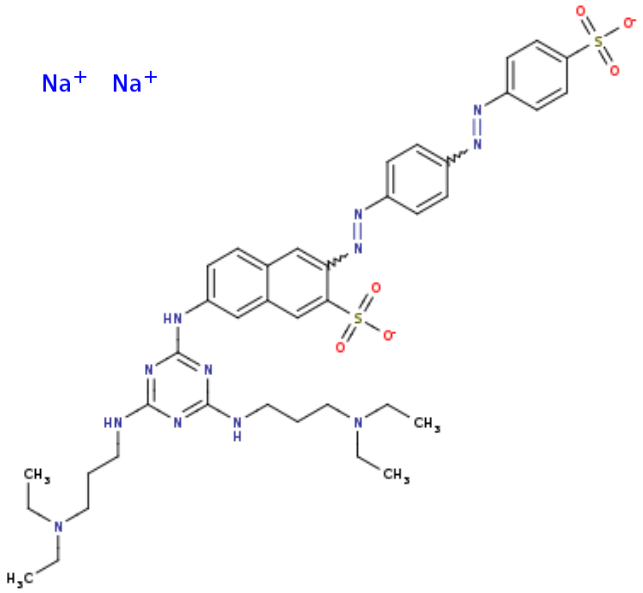
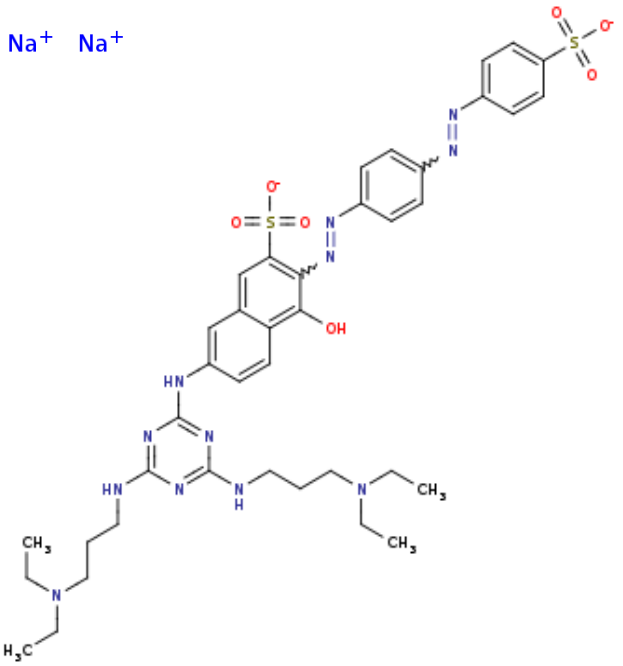
106028-58-4			EC number 405-150-4

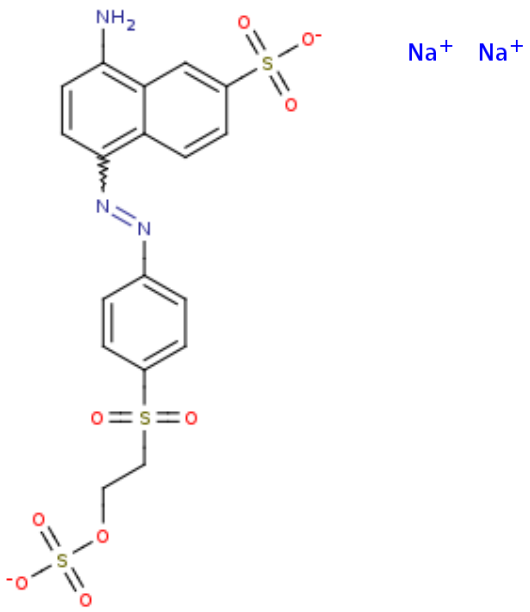
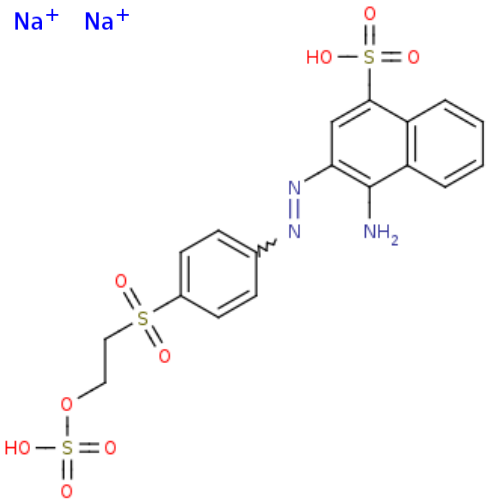
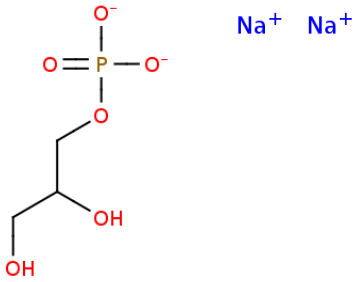
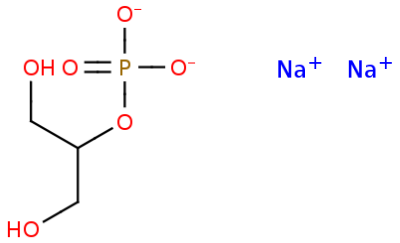
76508-02-6	  	 Na^+ Na^+ Na^+ Na^+ Na^+ Na^+	EC number 405-280-1 CAS RN™ includes only the second structure

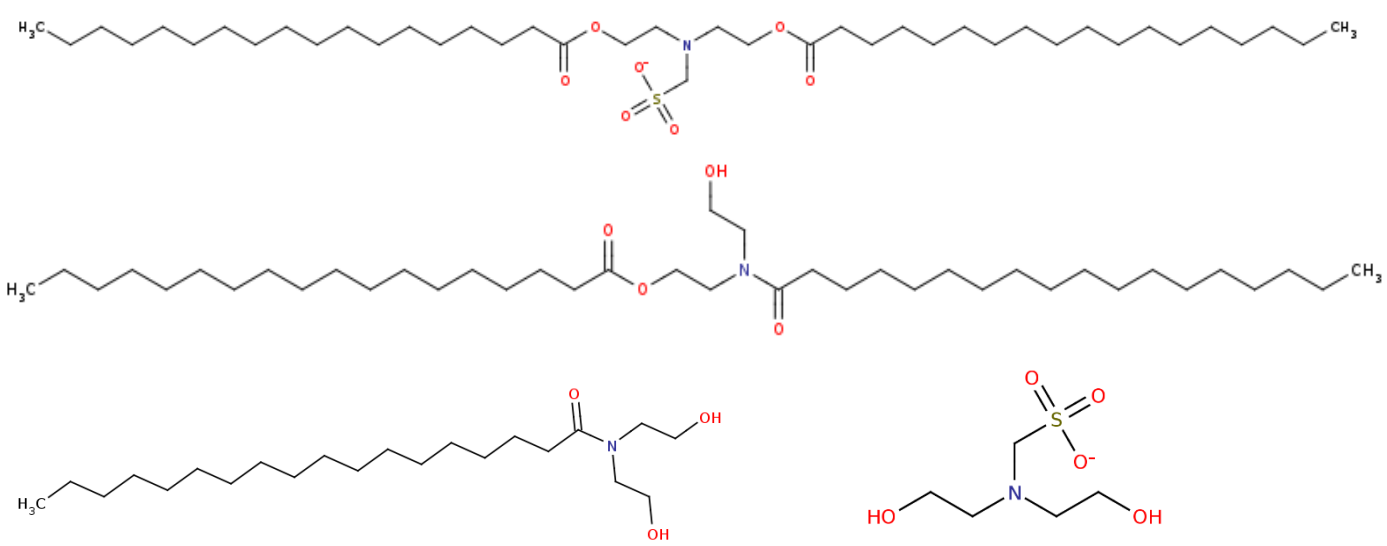
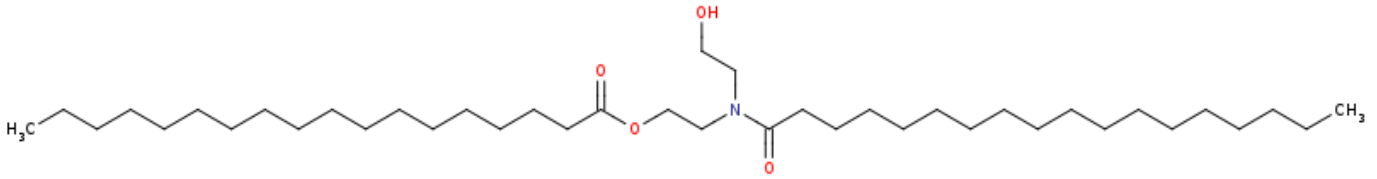
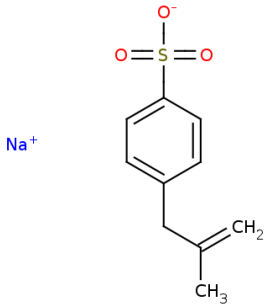
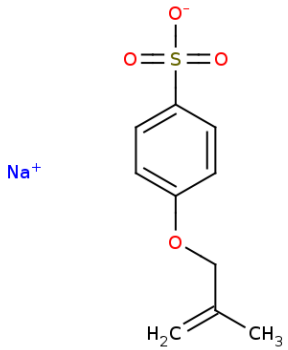
85153-92-0 (incorrect form)		EC number 400-050-7
85153-92-0 (correct form)		EC number 400-050-7

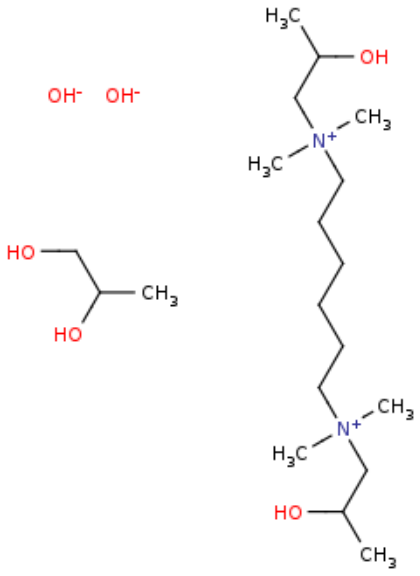
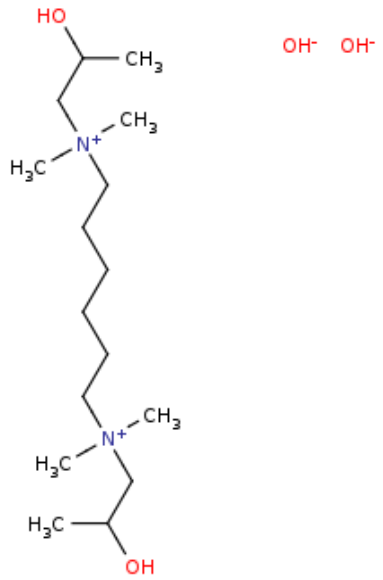
371921-41-4 (incorrect form)		EC number 429-230-3 'correct' form has still missing stereoinformation
371921-41-4 (correct form)		EC number 429-230-3 'correct' form has still missing stereoinformation

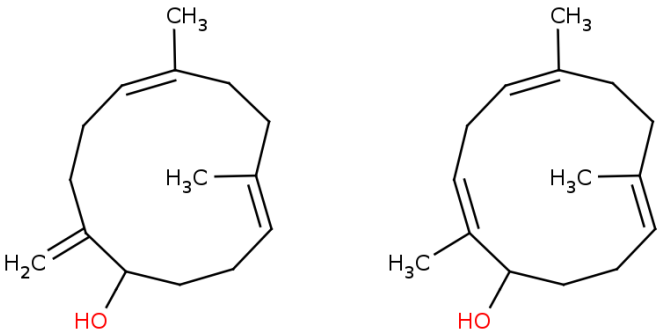
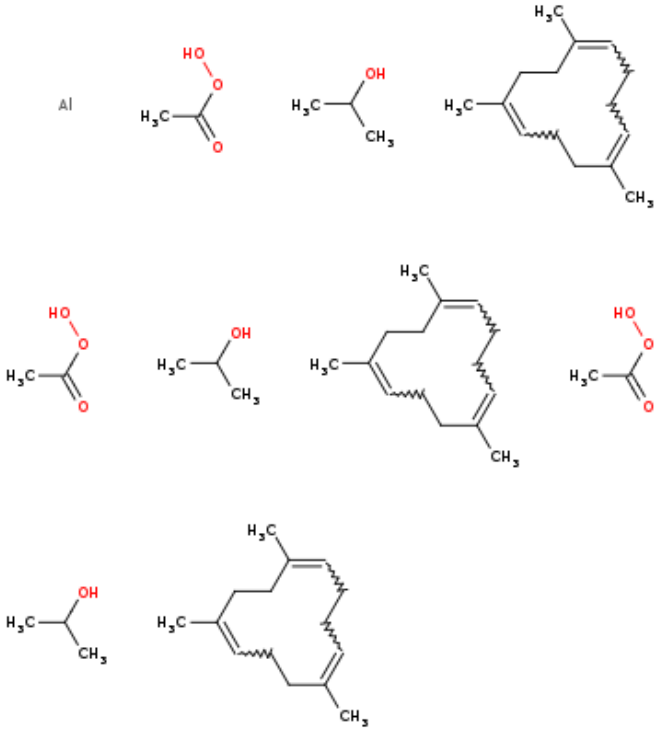
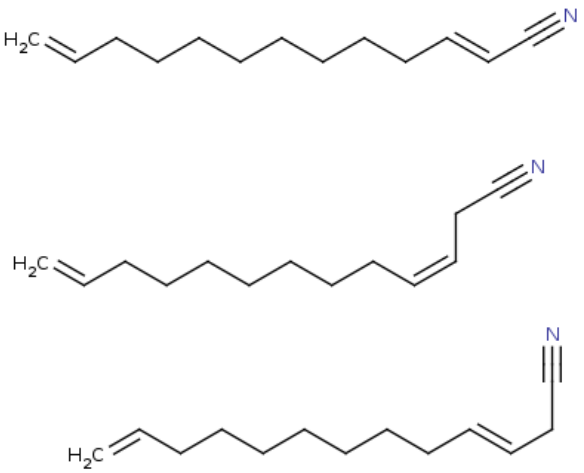
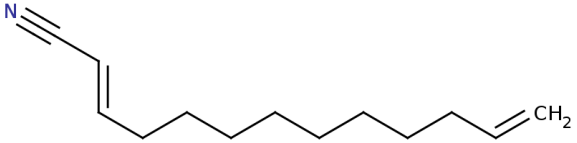
70161-14-7			EC number 274-349-4
72968-81-1			EC number 277-155-8

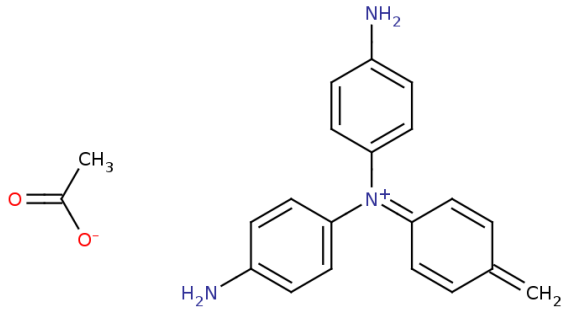
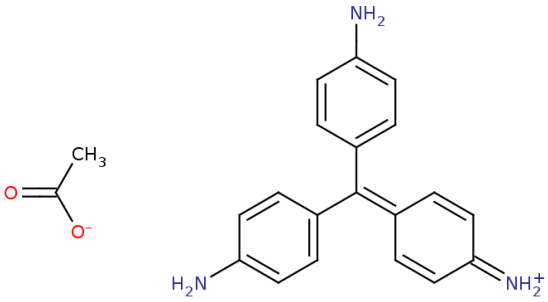
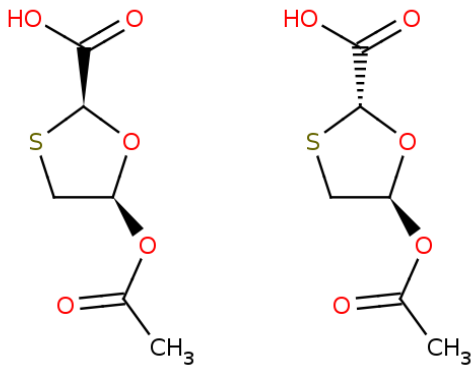
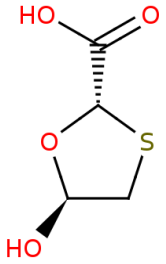
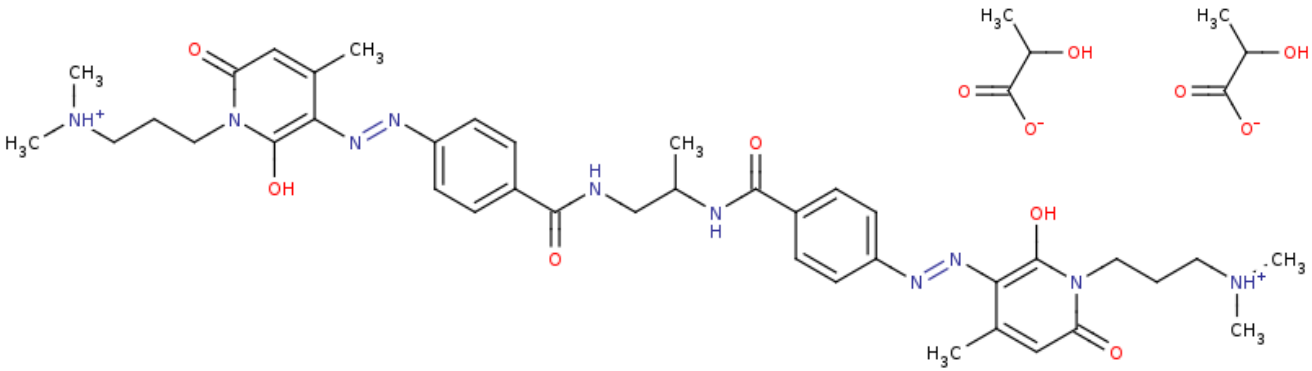
147703-64-8			EC number 410-390-8
120029-06-3			EC number 419-460-2

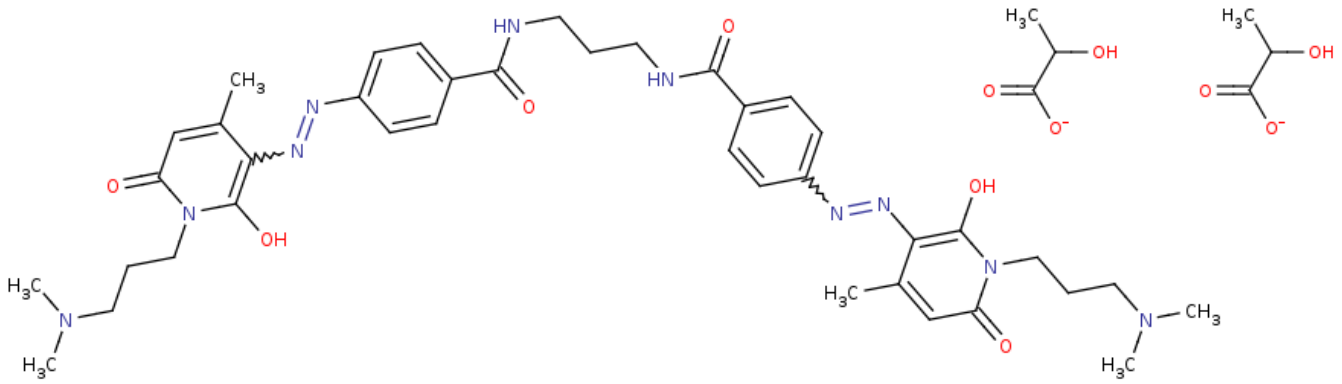
250688-43-8			EC number 423-730-5
819-83-0			EC number 212-464-3

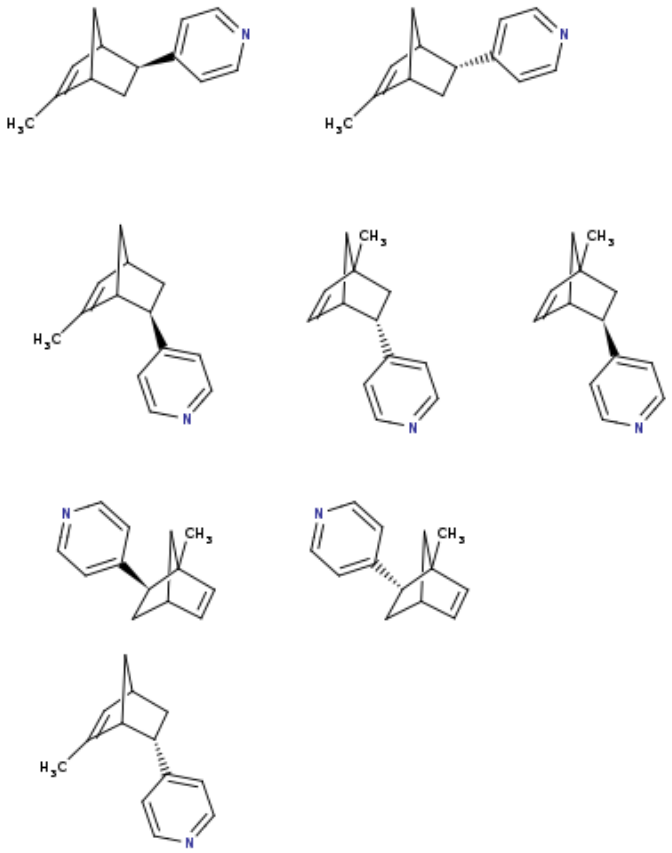
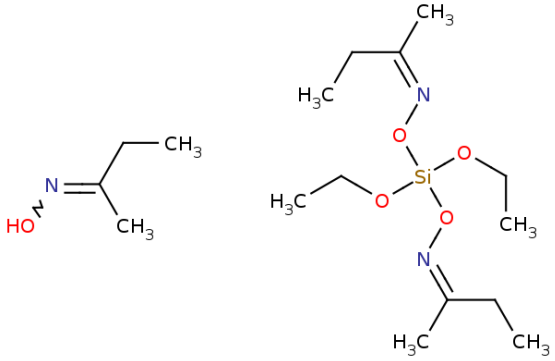
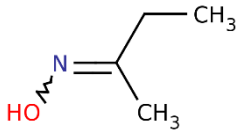
55349-70-7 (incorrect form)		EC number 401-230-8
55349-70-7 (correct form)		EC number 401-230-8 CAS no. contains only second structure
1208-67-9	 	EC number 214-901-3

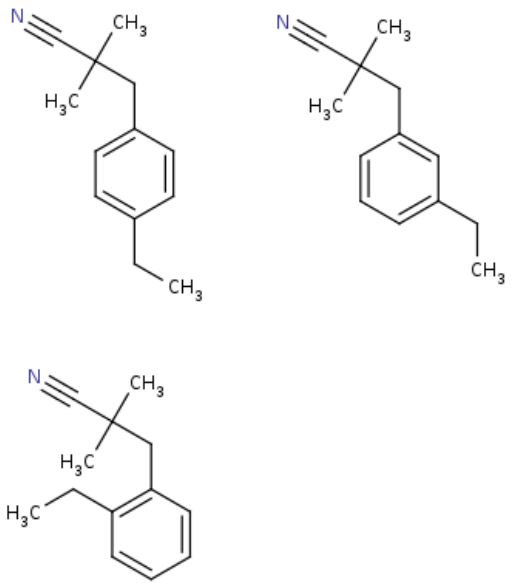
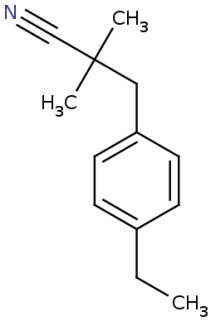
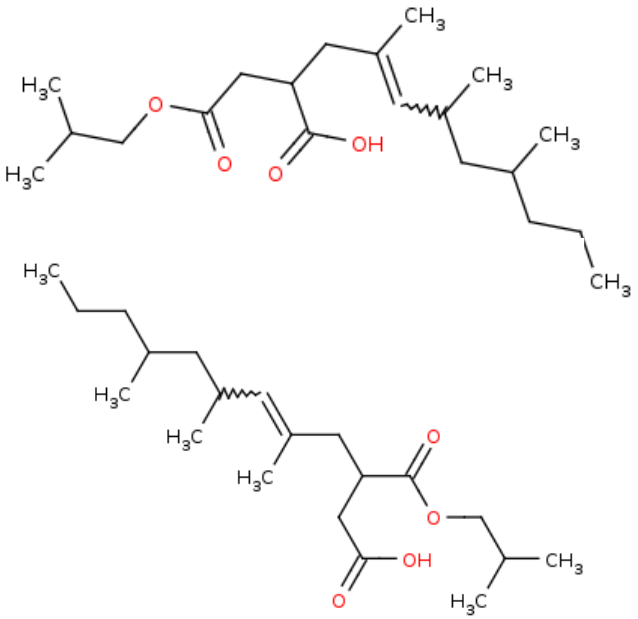
35132-93-5			EC number 442-730-6 CAS no. does not contain all structural elements

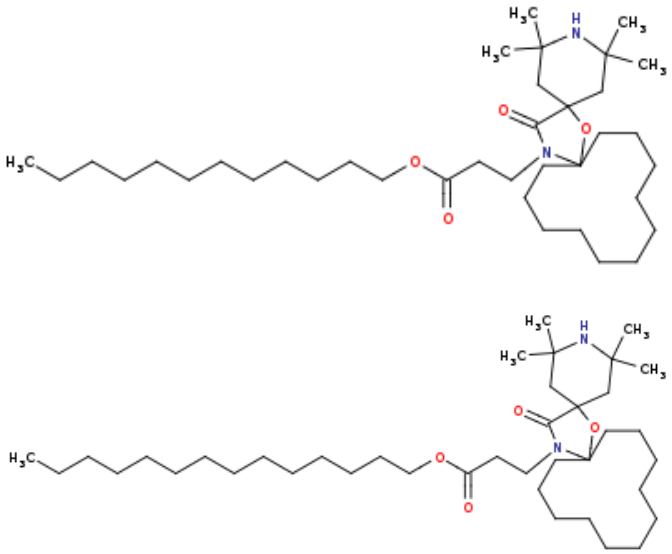
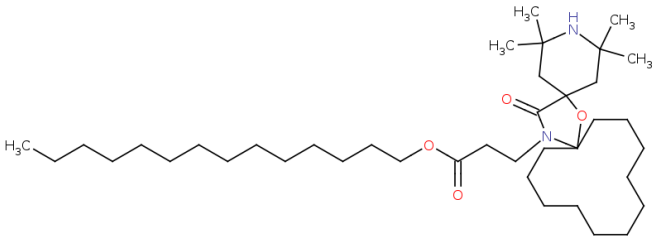
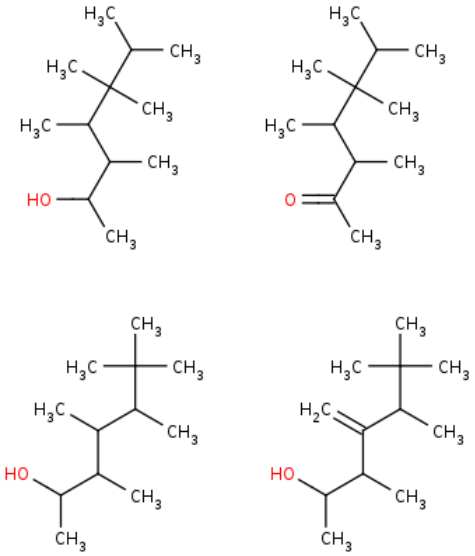
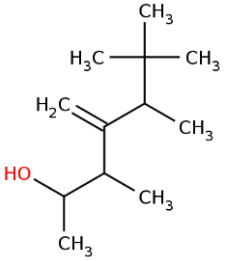
111850-00-1			EC number 413-530-6 'correct' form has still missing stereoinformation
124071-40-5			EC number 422-190-8 CAS RN™ contains only the first structure

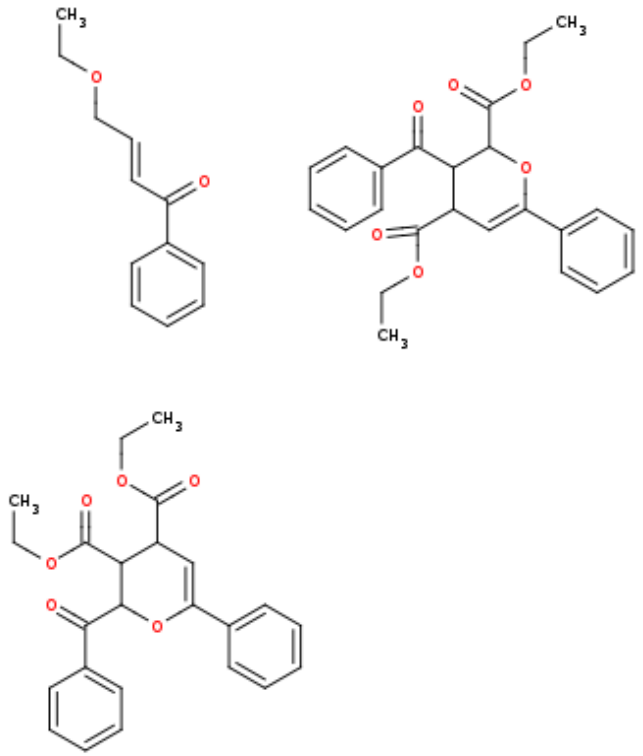
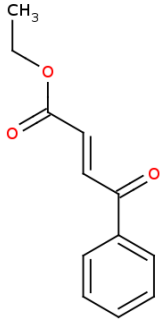
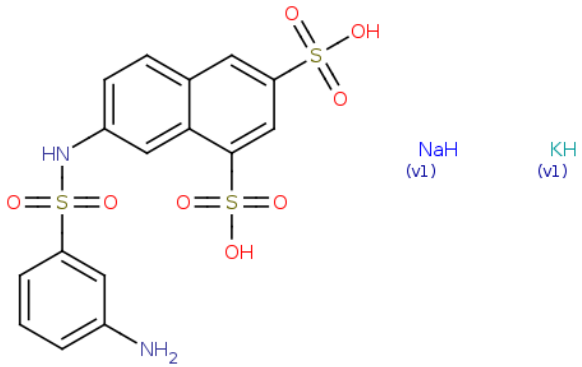
6035-94-5			EC number 227-918-6
147027-04-1			EC number 411-660-8
164578-09-0 (incorrect form)			EC number 403-340-1

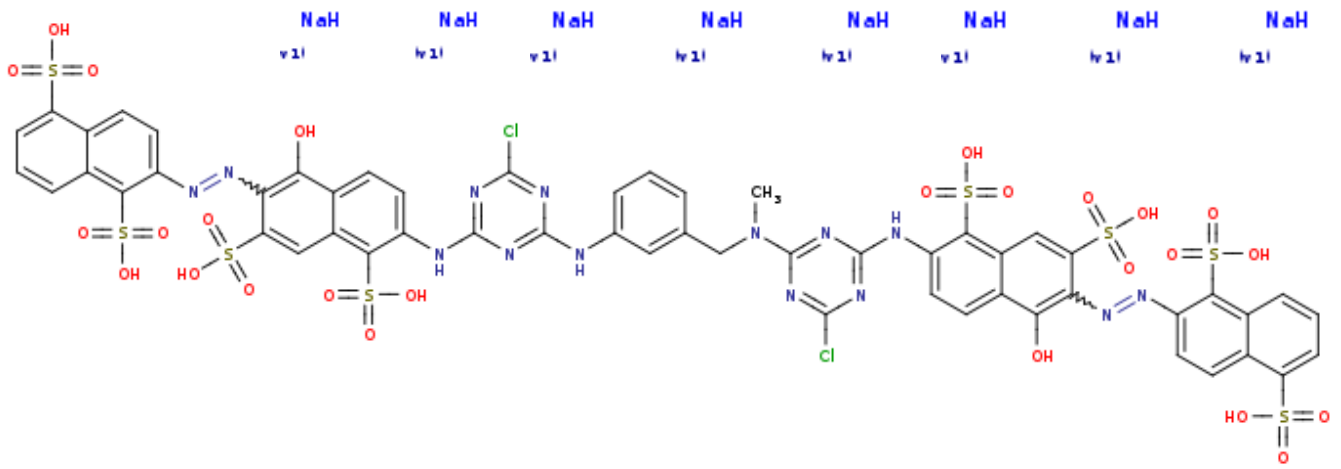
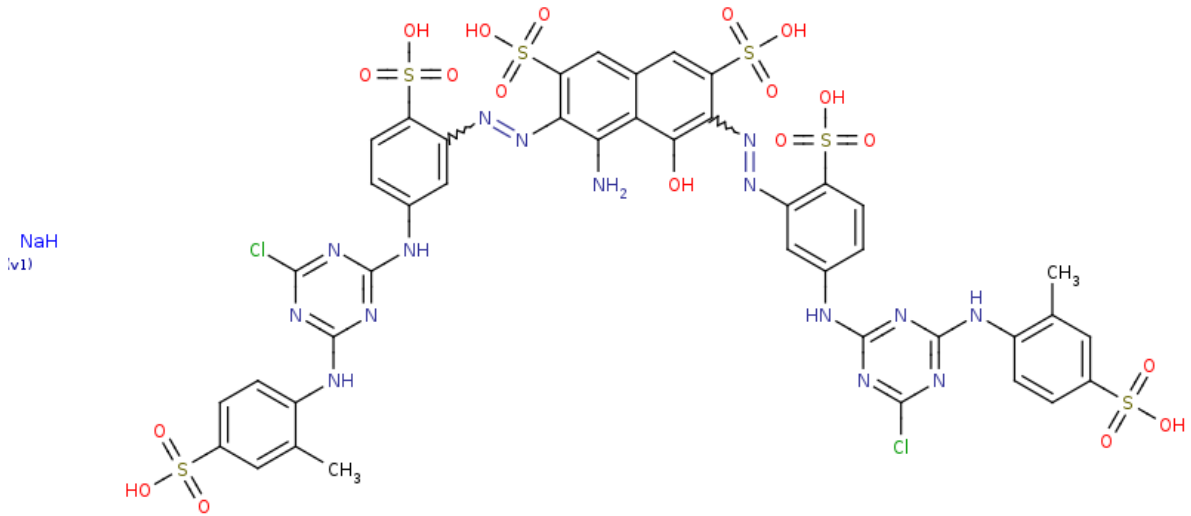
164578-09-0 (correct form)		EC number 403-340-1

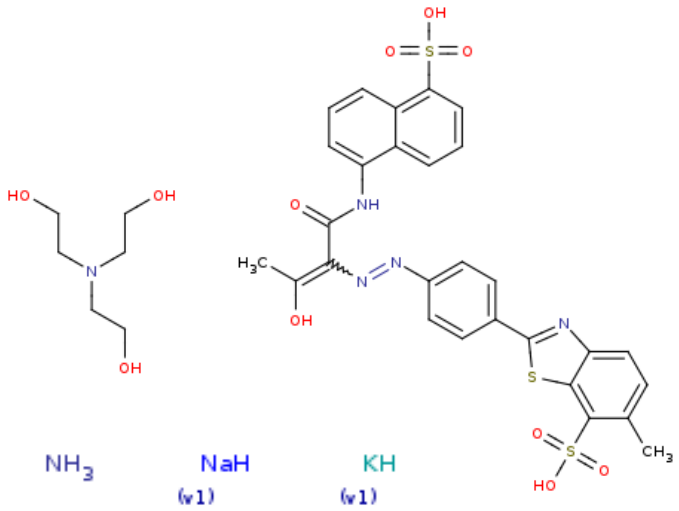
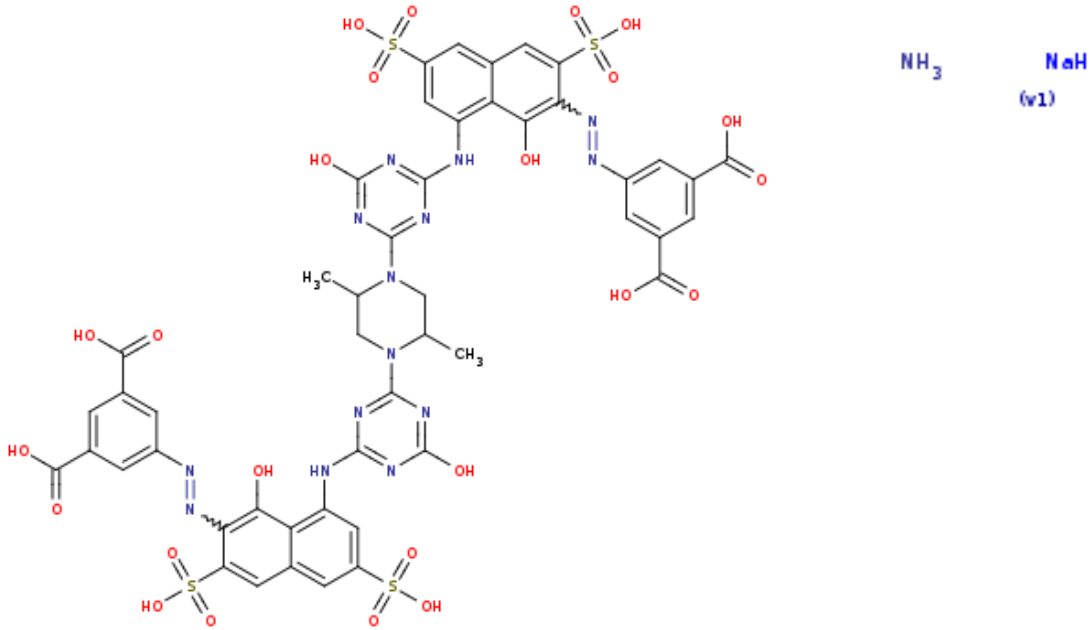
125352-06-9		The components shown in SciFinder do not correspond to the strucutre elemets shwon in the ECHA database. However, SciFinder has not the complete struture.	EC number 402-520-7
96-29-7			EC number 406-930-7

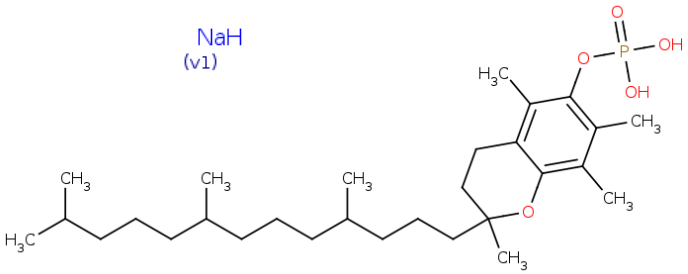
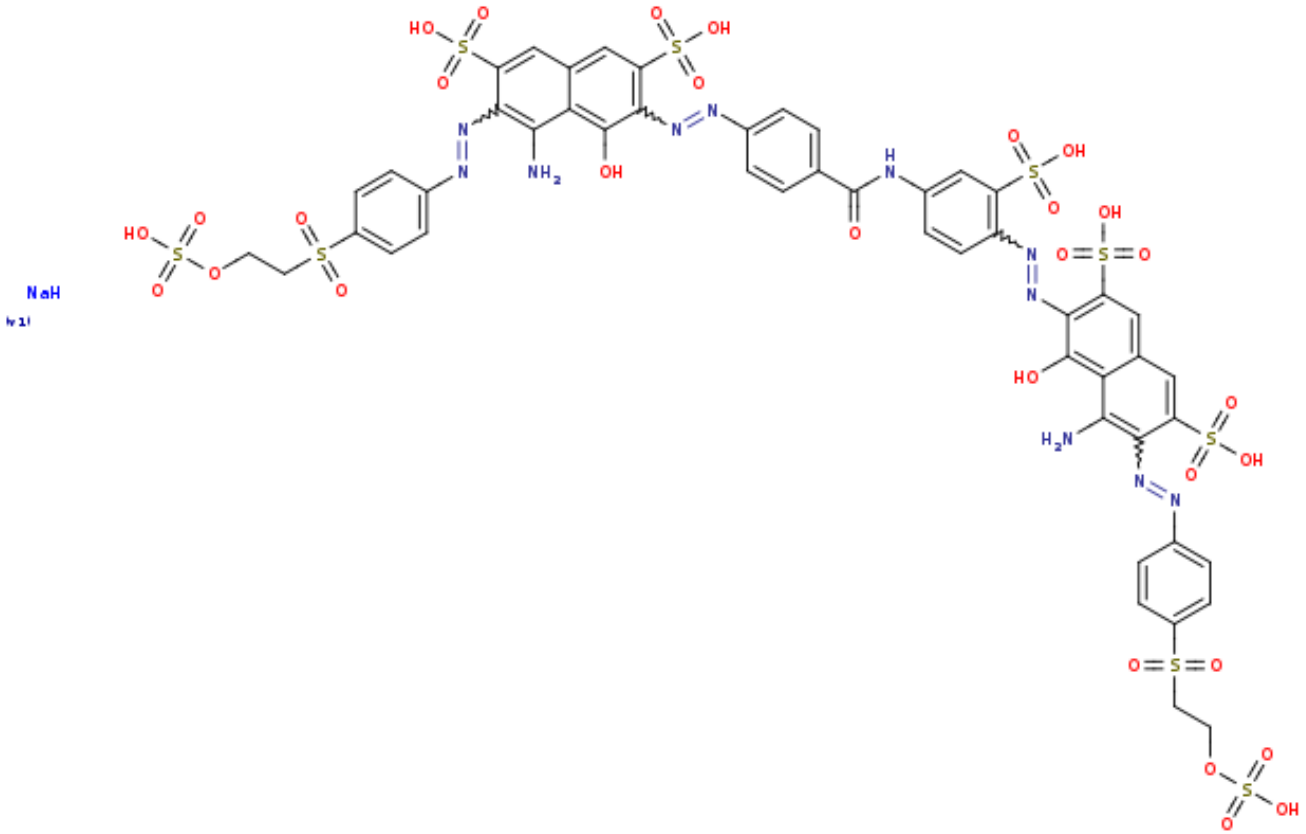
134123-93-6			EC number 412-660-0 CAS RN™ contains only the first structure
141847-13-4		SciFinder^{n} has no final structure but the components do not agree with the ones from the ECHA database	EC number 410-720-0

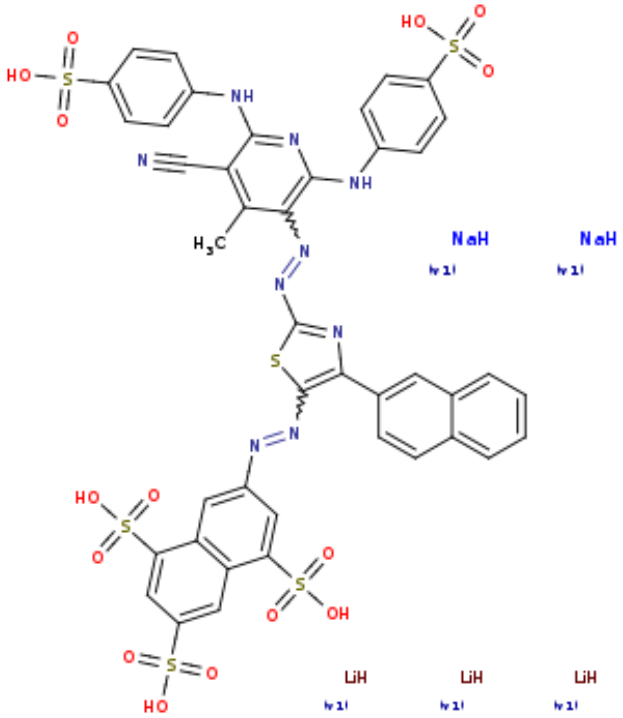
85099-50-9			EC number 400-580-9 CAS RN™ contains only the second structure
81787-06-6			EC number 401-030-0

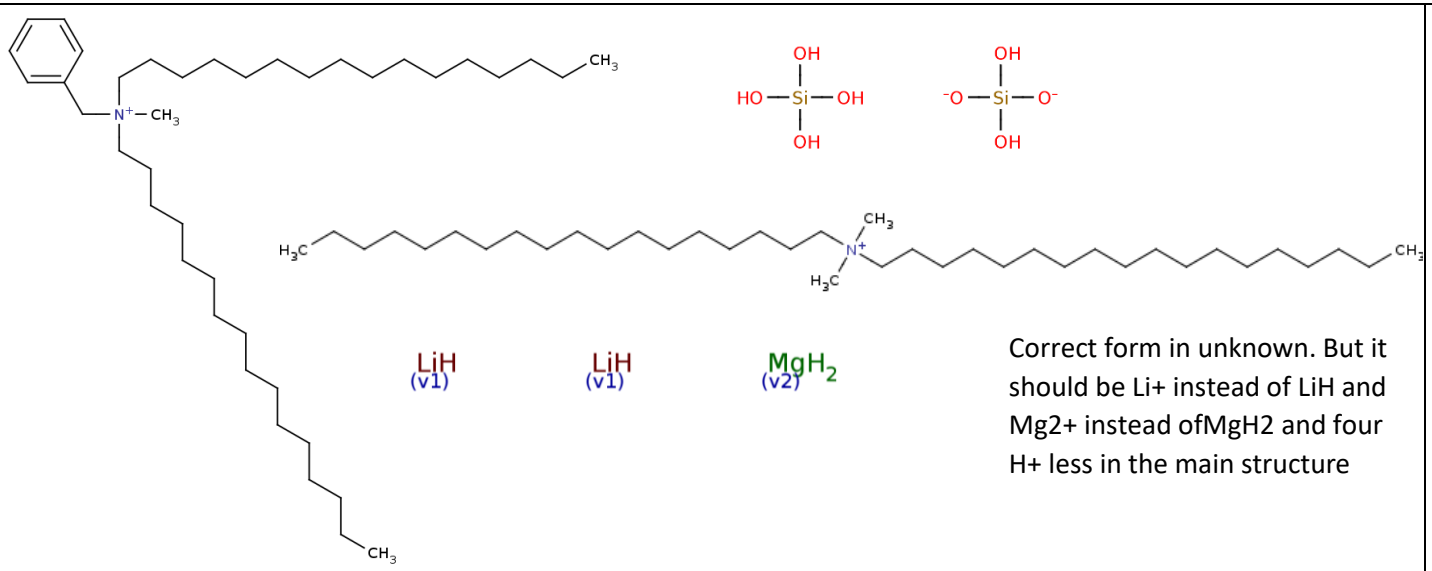
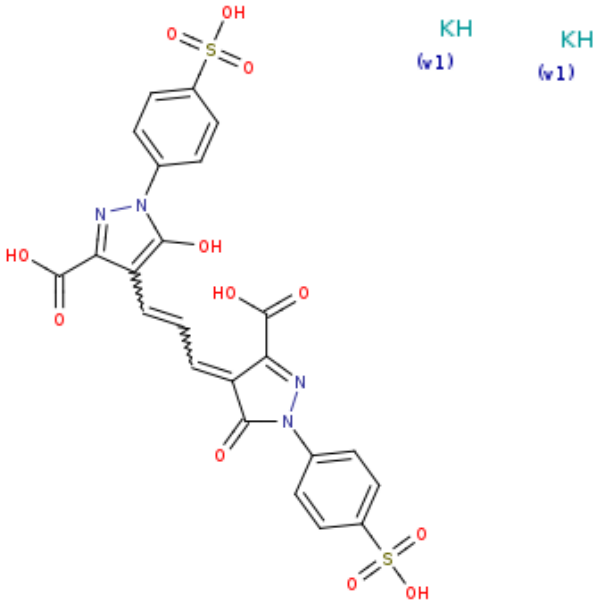
15121-89-8			EC number 438-510-4
-	 NaH (v1) KH (v1)	Correct form in unknown. But it should be Na+ instead of NaH and K+ instead of KH and two H+ less in the main structure	EC number 410-065-0

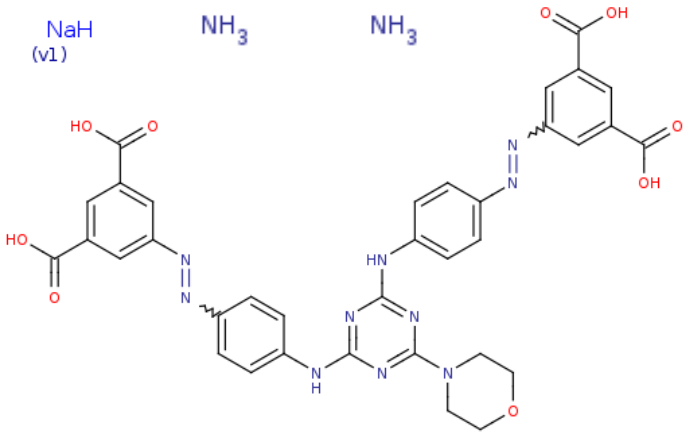
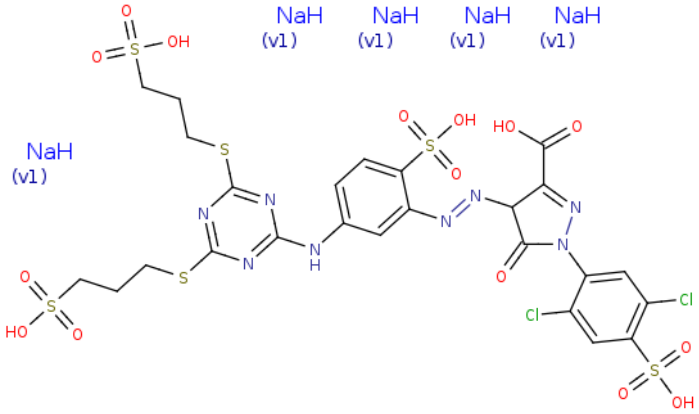
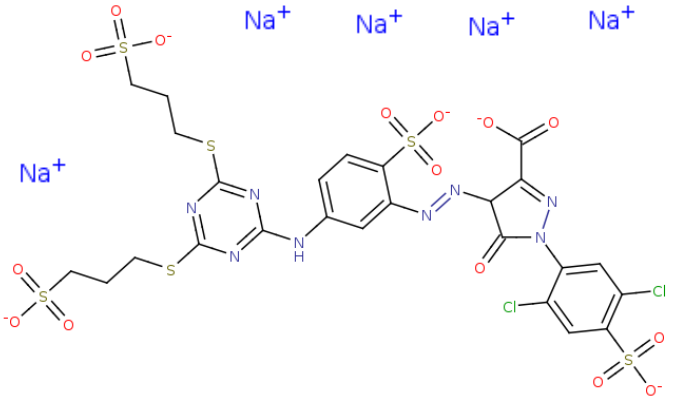
148878-21-1 (incorrect form)		EC number 412-960-1
148878-21-1 (correct form)	Correct form in unknown. But it should be Na+ instead of NaH and eight H+ less in the main structure	EC number 412-960-1
141250-43-3 (incorrect form)		EC number 435-350-7
141250-43-3 (correct form)	Correct form in unknown. But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

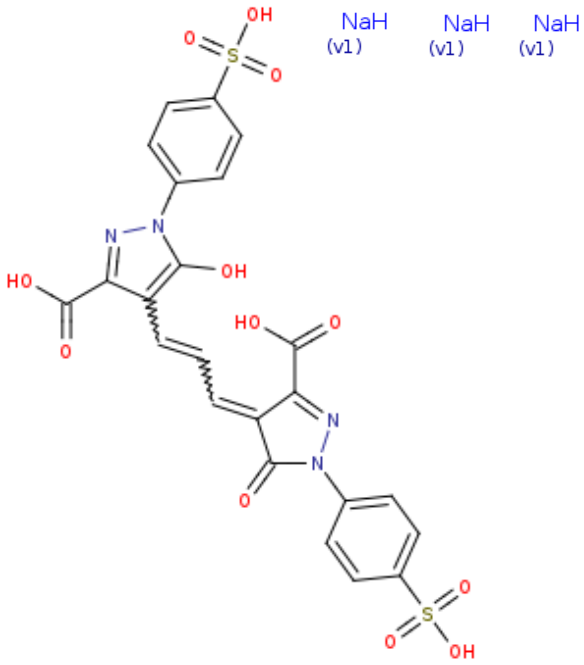
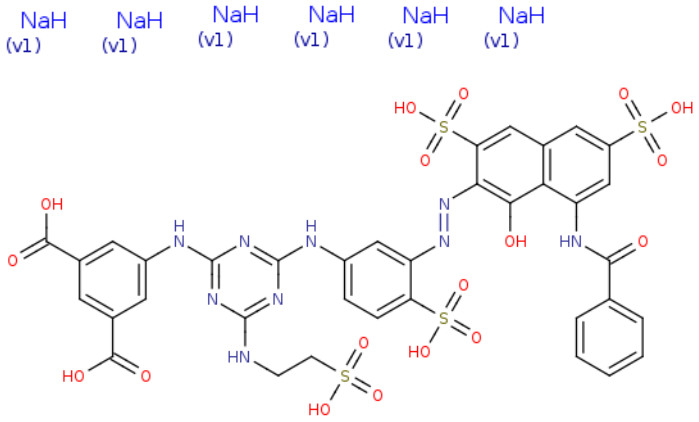
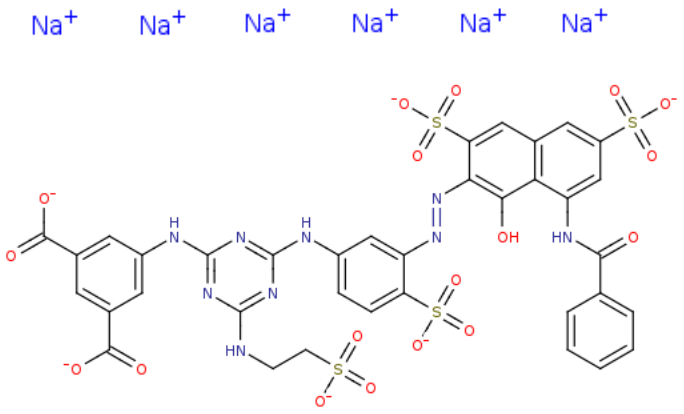
-		Correct form in unknown. But it should be Na+ instead of NaH and K+ instead of KH and two H+ less in the main structure	EC number 400-940-5
187285-15-0 (incorrect form)			EC number 413-180-4

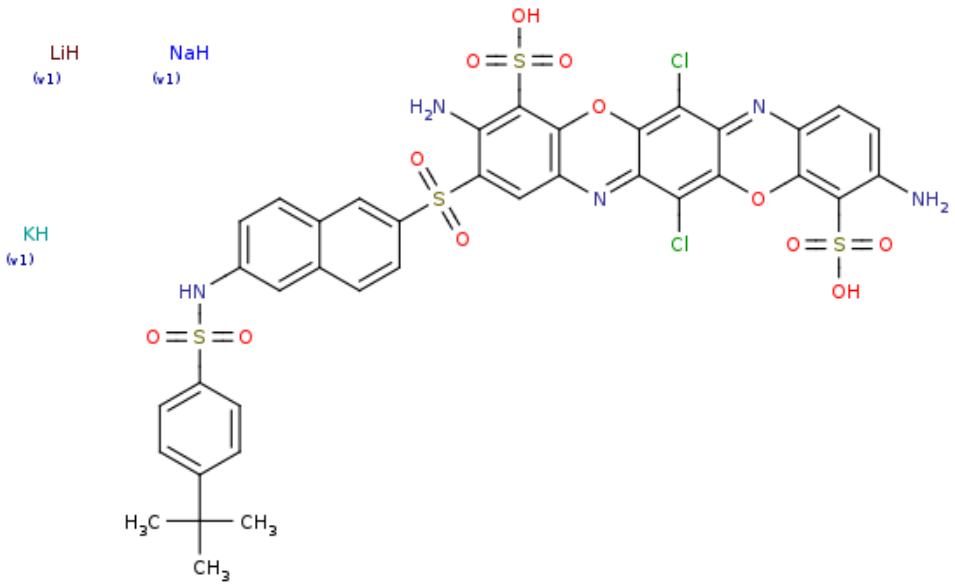
187285-15-0 (correct form)	Correct form in unknown. But it should be Na+ instead of NaH and one H+ less in the main structure		EC number 413-180-4
299158-63-7		Correct form in unknown. But it should be Na+ instead of NaH and one H+ less in the main structure	EC number 478-070-0
161935-19-9 (incorrect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

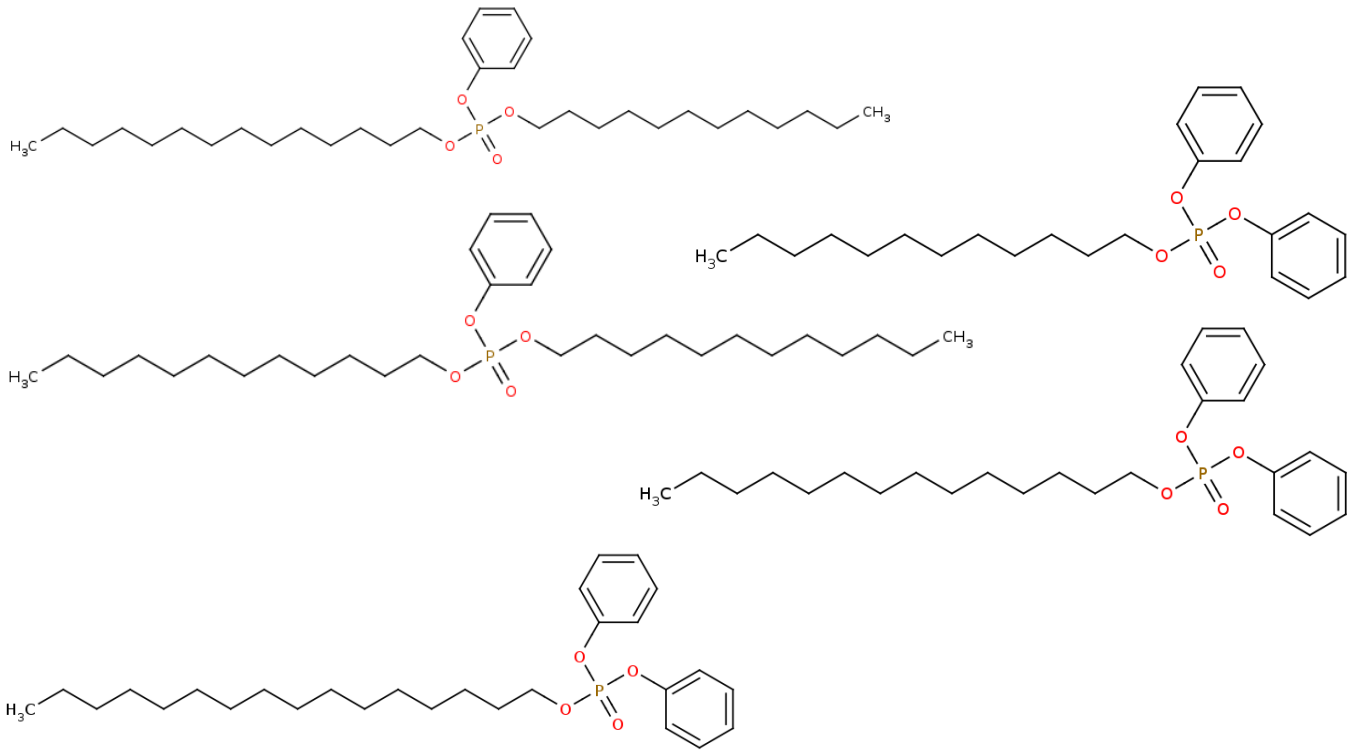
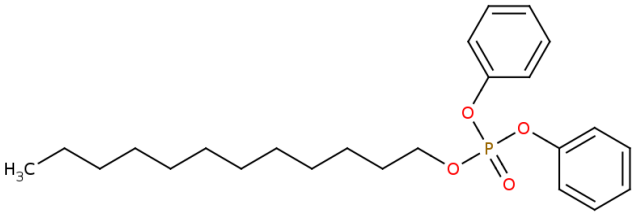
161935-19-9 (correct form)	Correct form in unknown. But it should be Na+ instead of NaH and one H+ less in the main structure		EC number 417-640-5
1016986-95-0		Correct form in unknown. But it should be Na+ instead of NaH and Li+ instead of LiH and five H+ less in the main structure	EC number 471-980-9

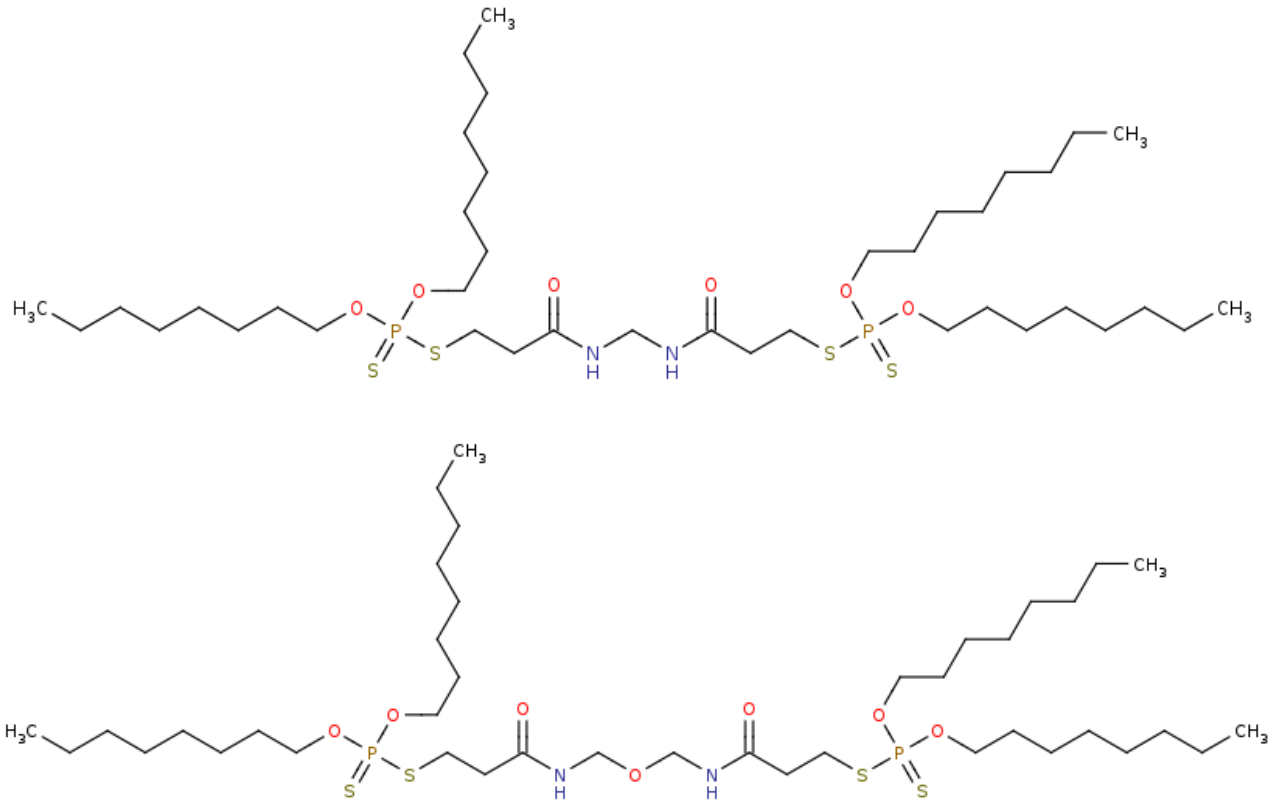
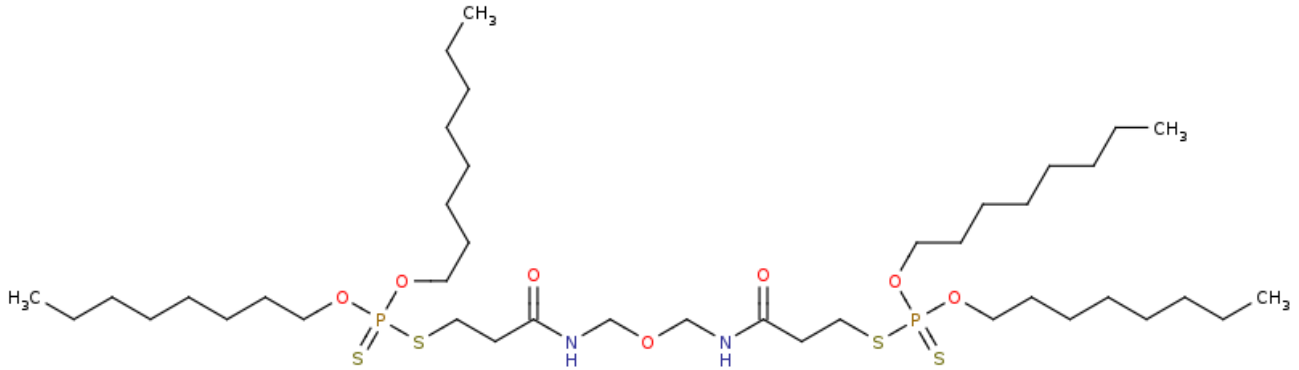
130500-97-9 (incorrect form)		Correct form in unknown. But it should be Li+ instead of LiH and Mg2+ instead ofMgH2 and four H+ less in the main structure	EC number 401-480-8
-		Correct form in unknown. But it should beK+ instead of KH and 2 H+ less in the main structure	EC number 418-910-5

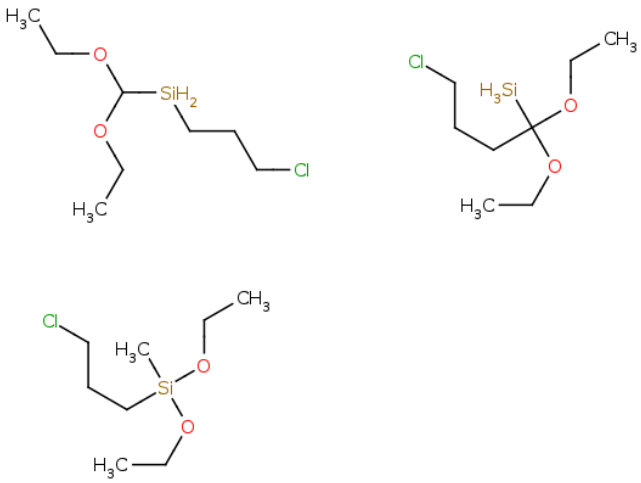
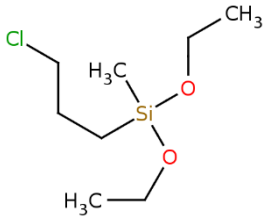
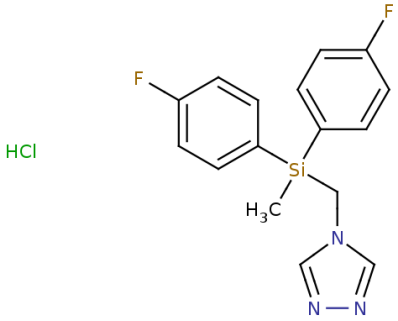
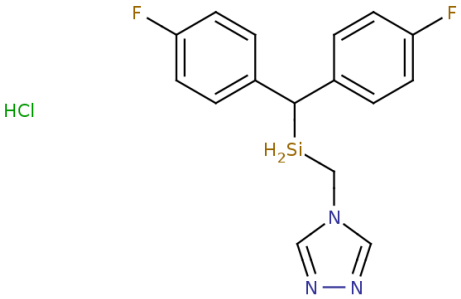
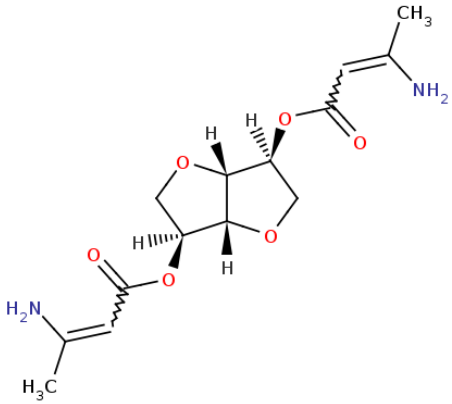
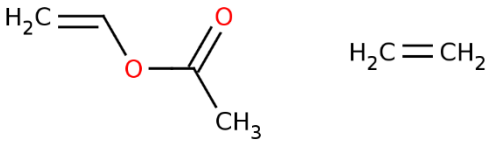
1379676-83-1		Correct form in unknown. But it should be Na+ instead of NaH and one H+ less in the main structure	EC number 414-410-6
187674-76-6			EC number 456-170-5

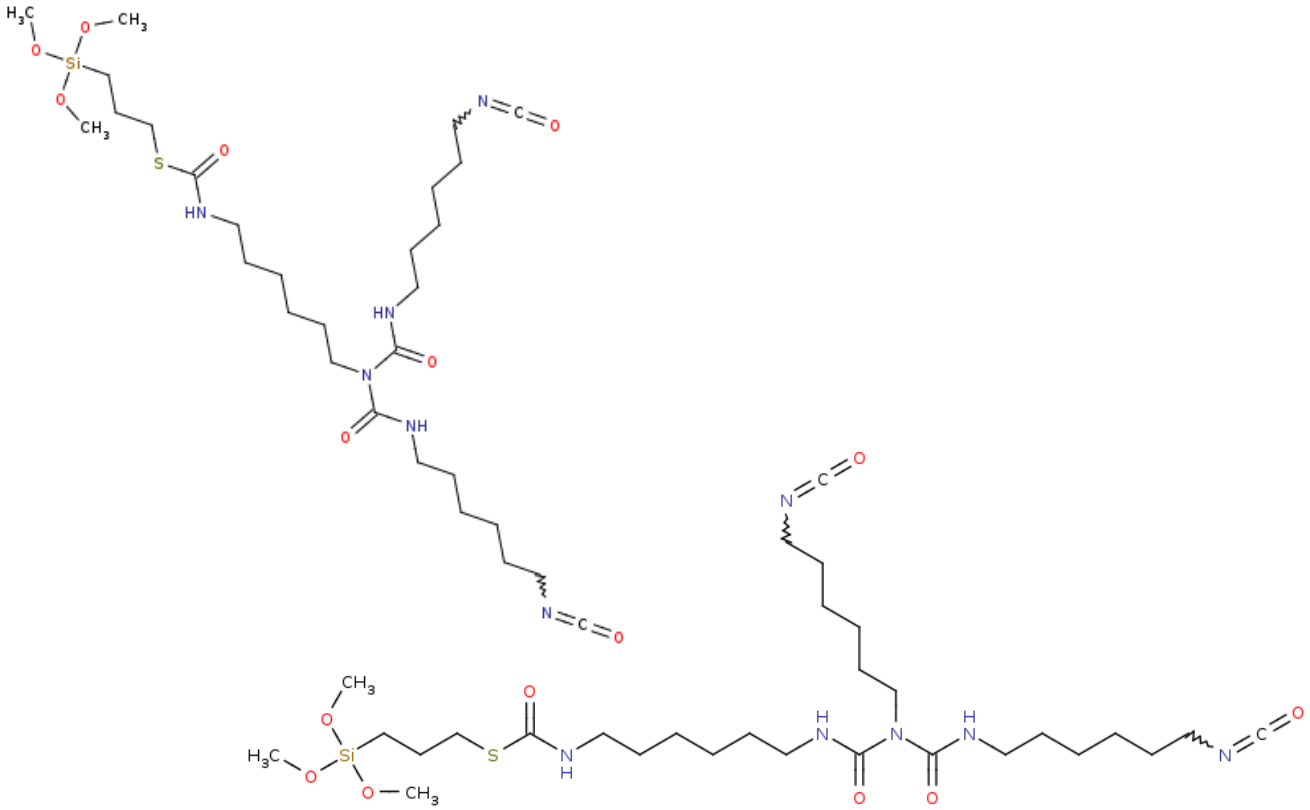
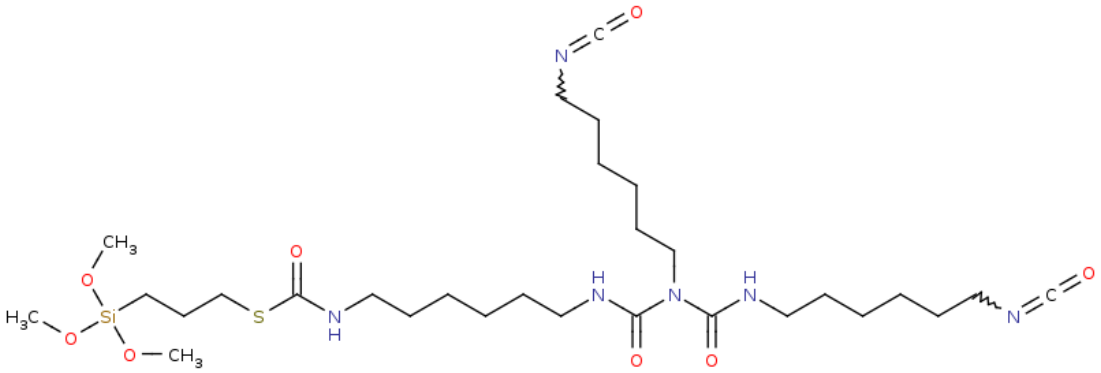
		Correct form in unknown. But it should be Na+ instead of NaH and three H+ less in the main structure	EC number 426-690-7
			EC number 482-150-0

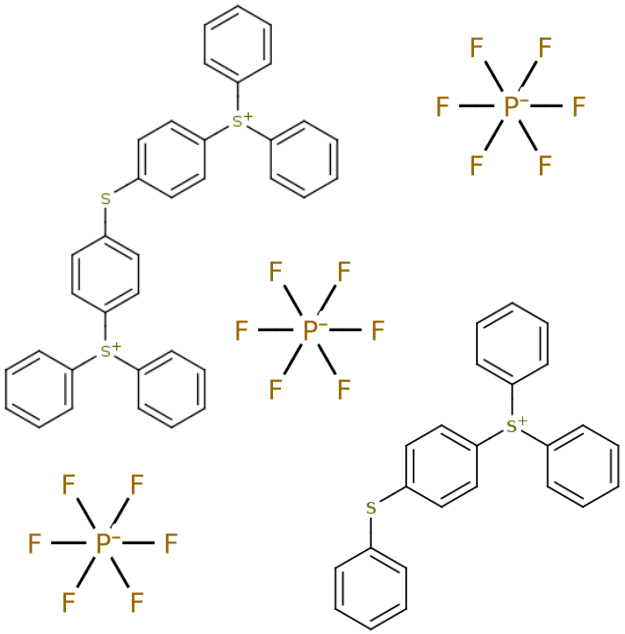
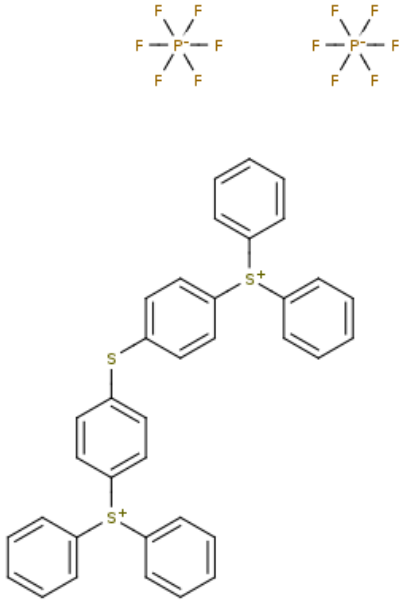
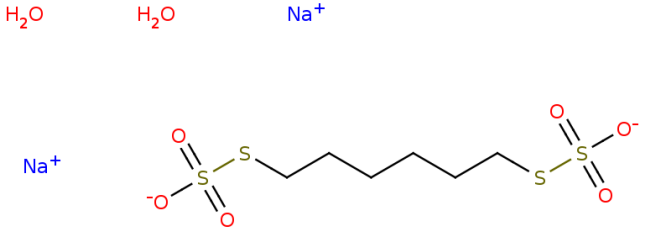
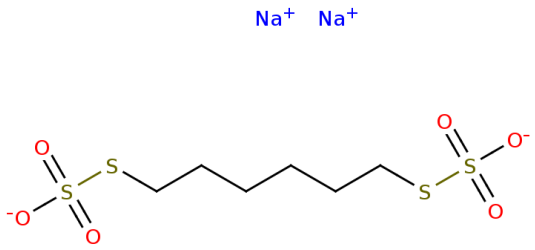
371921-63-0 (incorrect form)		EC number 440-770-9
371921-63-0 (correct form)	Correct form in unknown. But it should be Na+ instead of NaH, K+ instead of KH, and Li+ instead of LiH and three H+ less in the main structure	

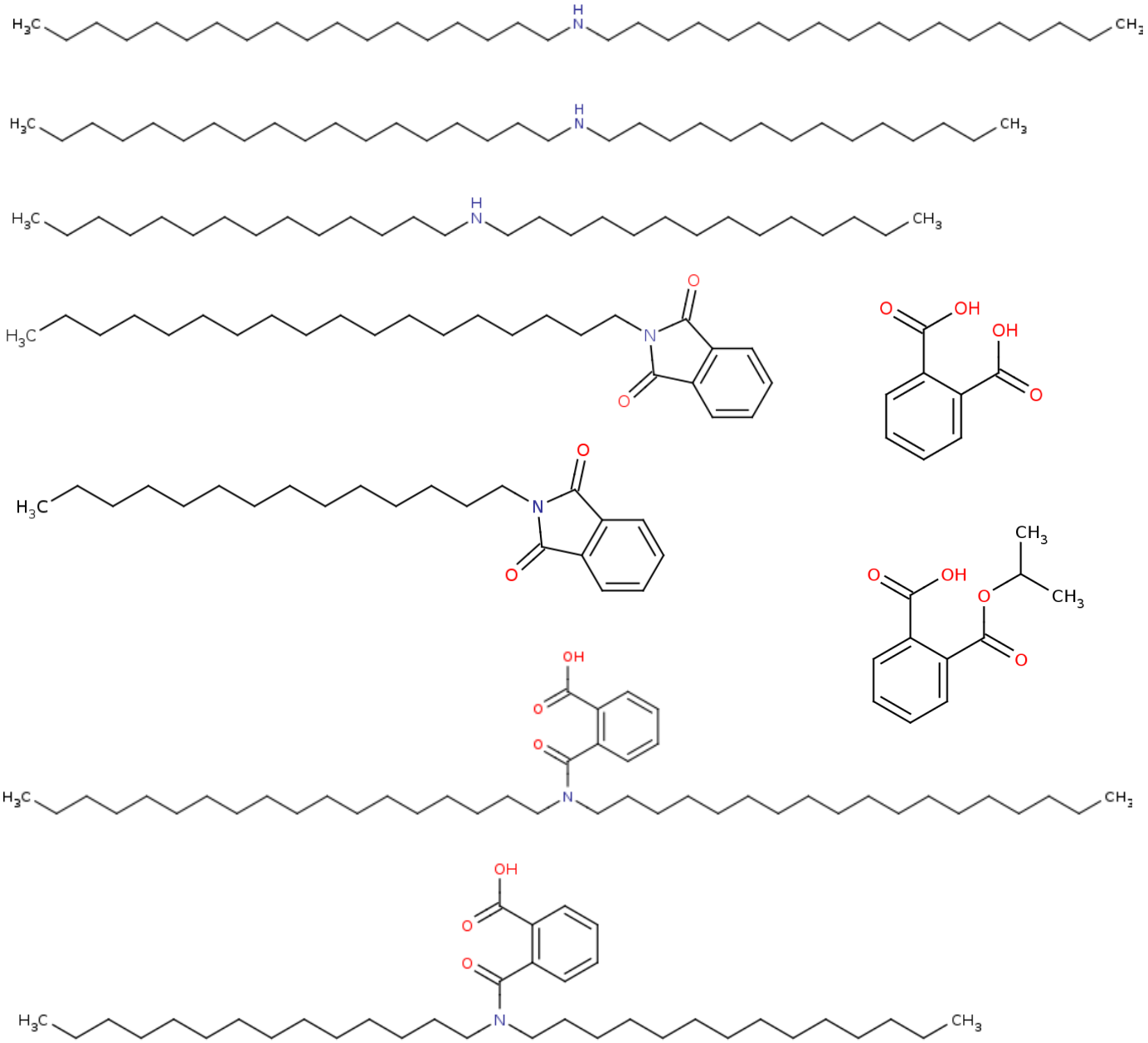
27460-02-2 (incorrect form)		EC number 431-760-5
27460-02-2 (correct form)		EC number 431-760-5 CAS contains only one of the structures

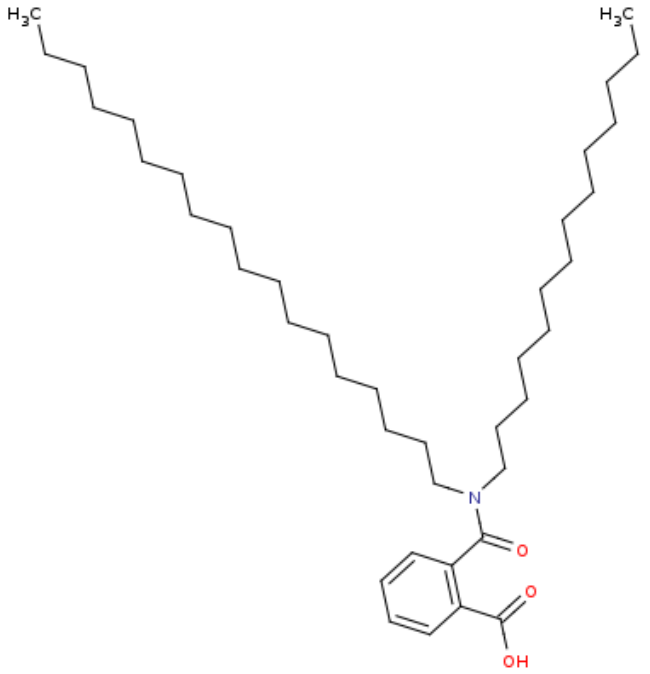
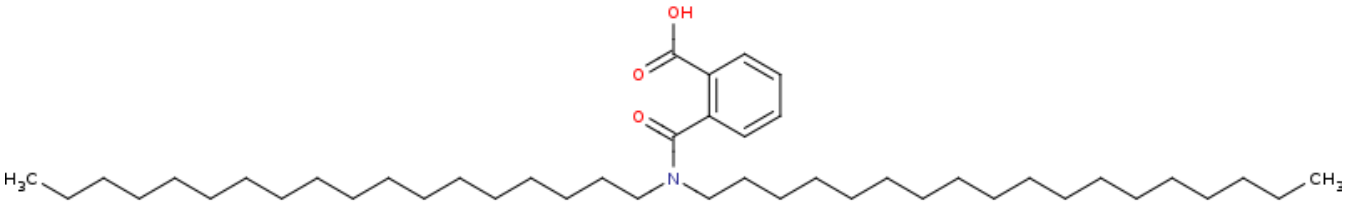
793710-14-2 (incorrect form)		EC number 401-820-5
793710-14-2 (correct form)		EC number 401-820-5 CAS RN™ contains only the second structure

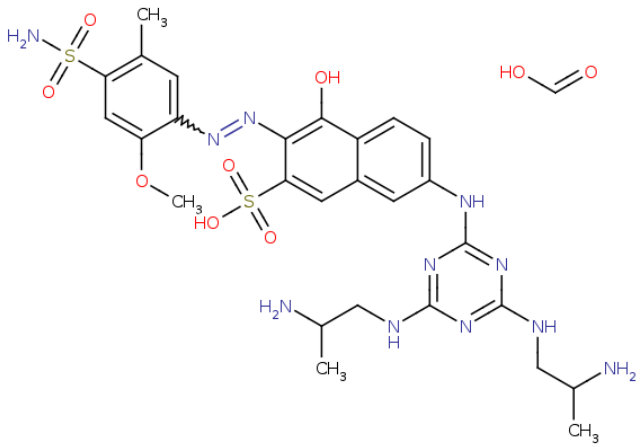
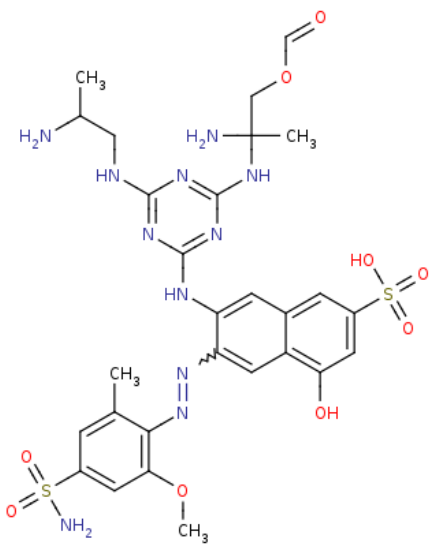
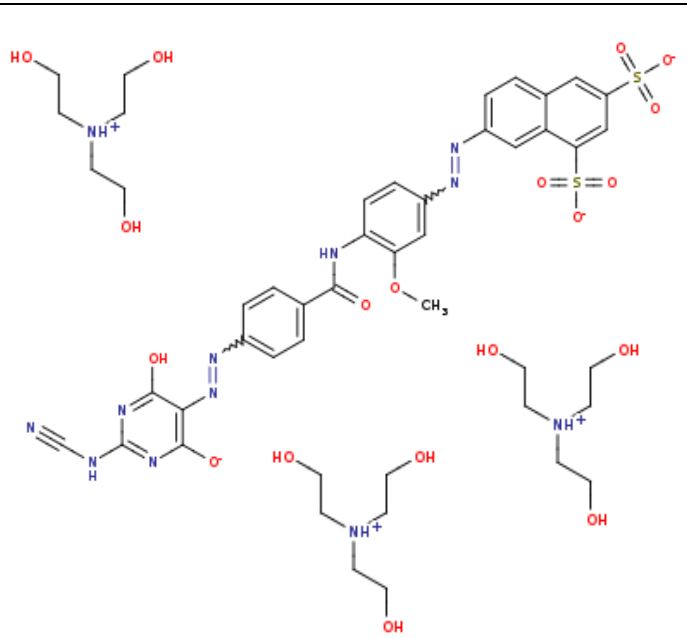
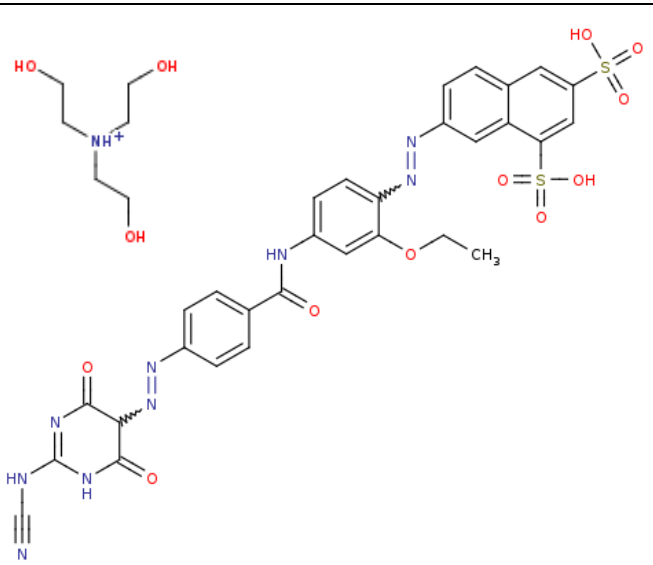
13501-76-3			EC number 236-828-6 CAS RN™ contains only the third structure
89066-61-5			EC number 401-380-4
24937-78-8			EC number 429-840-1

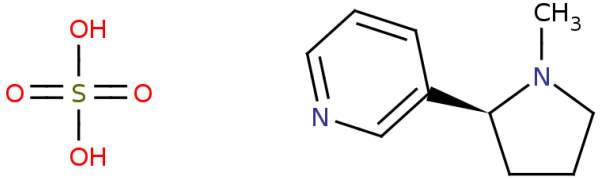
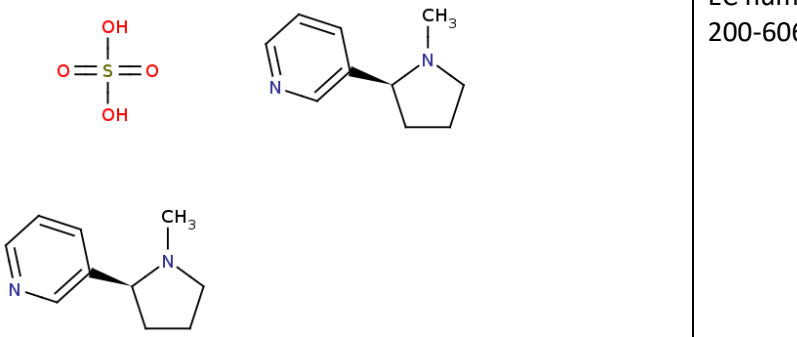
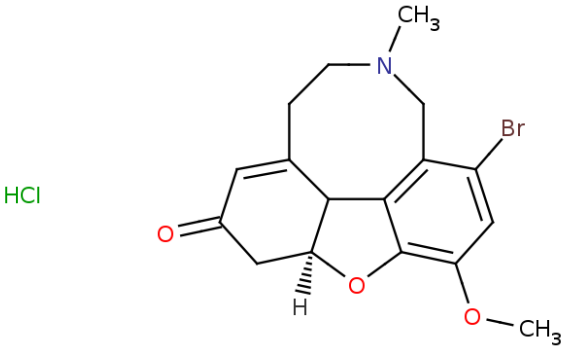
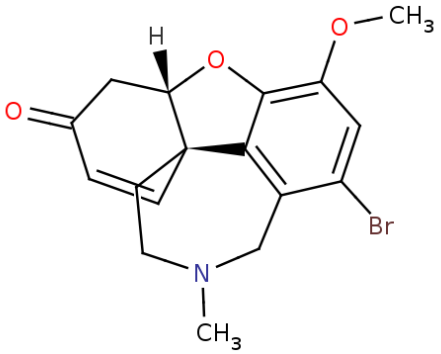
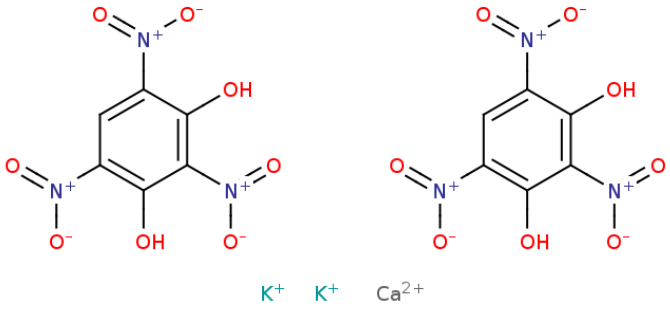
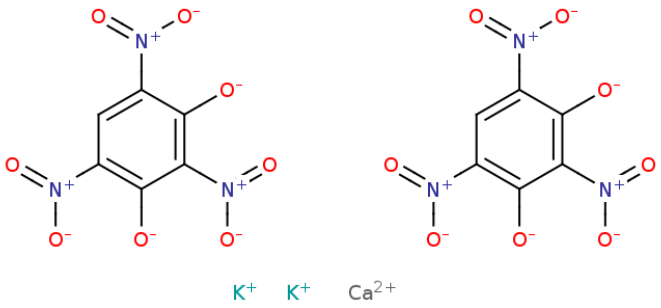
85702-90-5 (incorrect form)		EC number 402-290-8
85702-90-5 (correct form)		EC number 402-290-8 CAS RN™ contains only the second structure

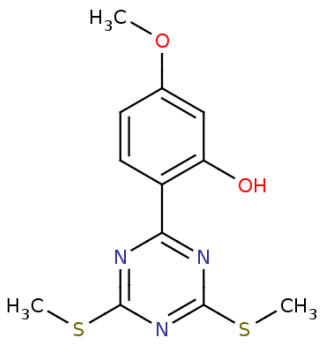
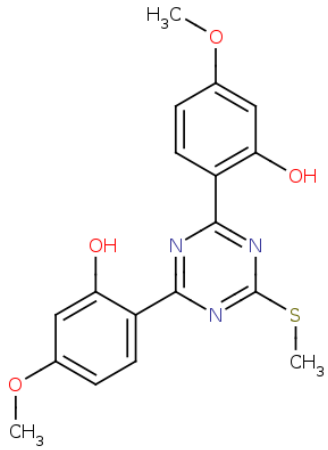
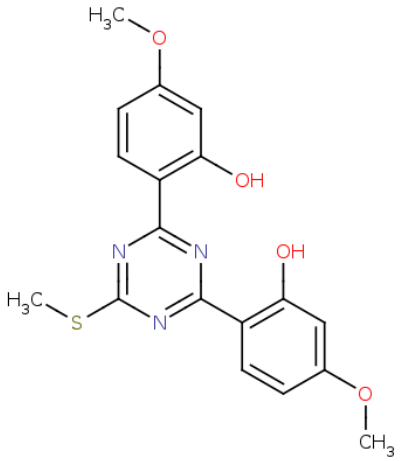
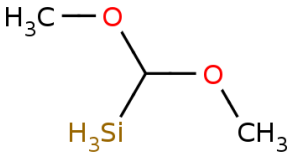
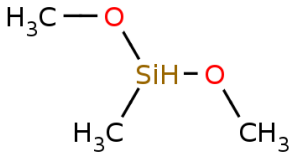
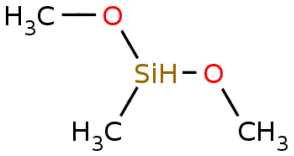
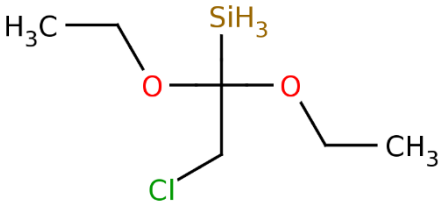
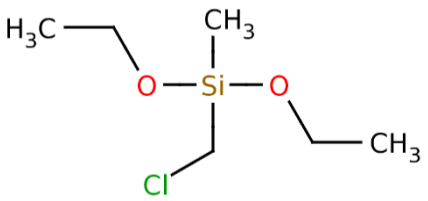
74227-35-3			EC number 404-986-7 CAS RN™ does not contain all structural elements
5719-73-3			EC number 401-320-7

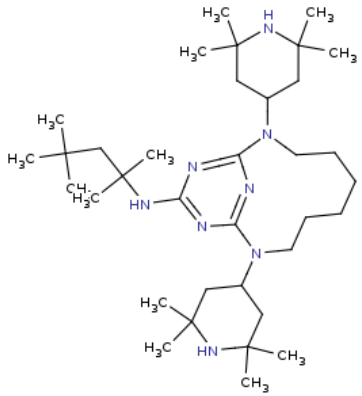
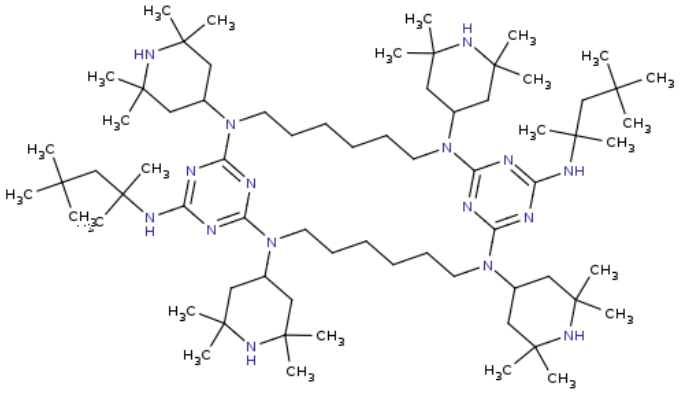
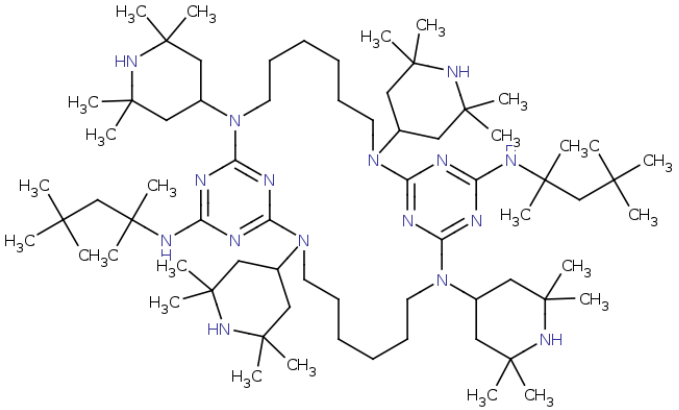
87787-81-3 (incorrect from part 1)		EC number 413-800-3

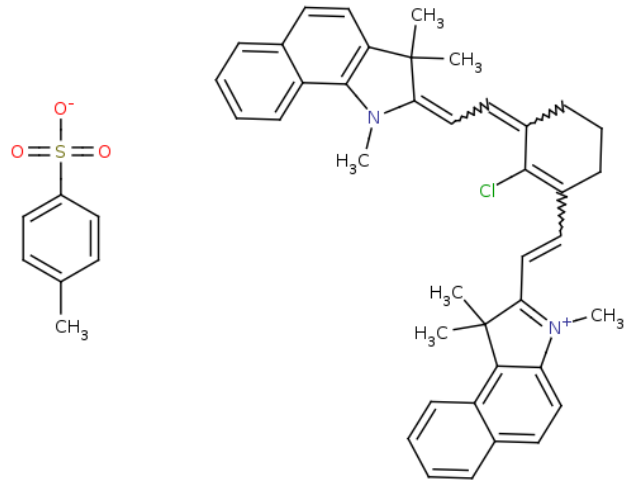
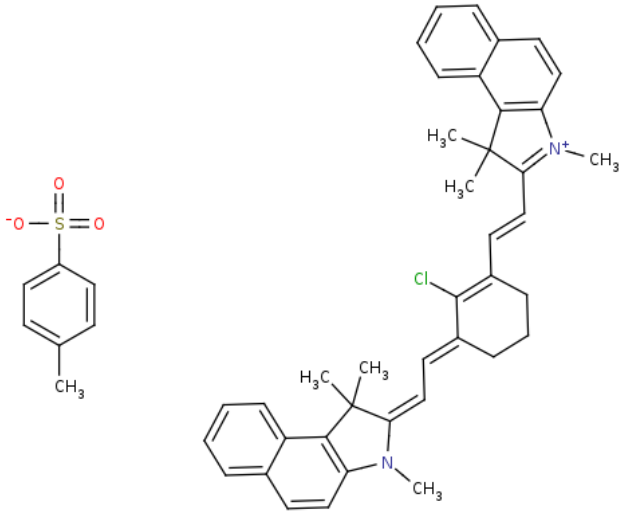
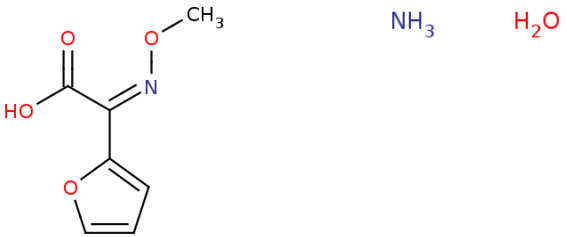
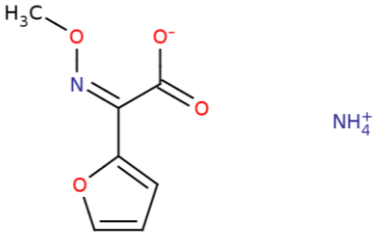
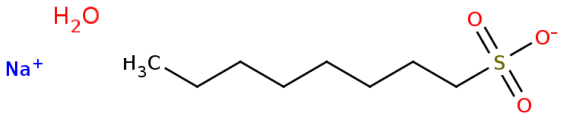
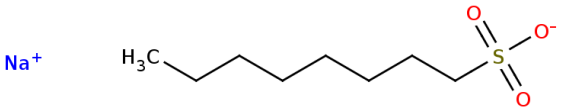
87787-81-3 (incorrect from part 2)		EC number 413-800-3
87787-81-3 (correct from)		EC number 413-800-3 CAS does not contain all structural elements

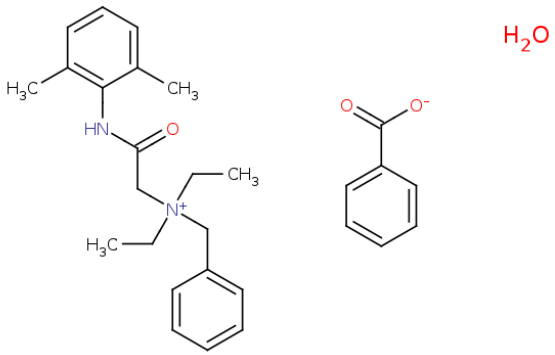
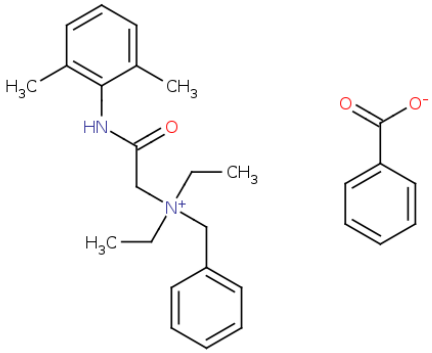
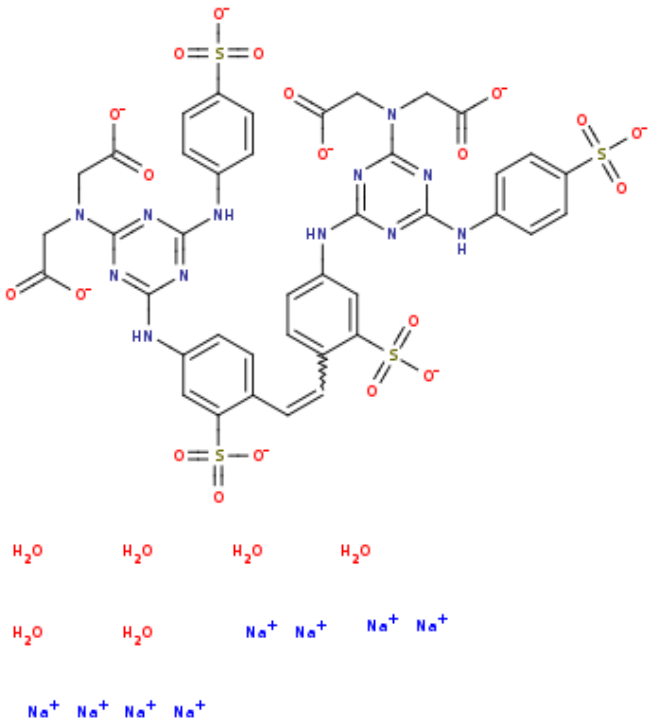
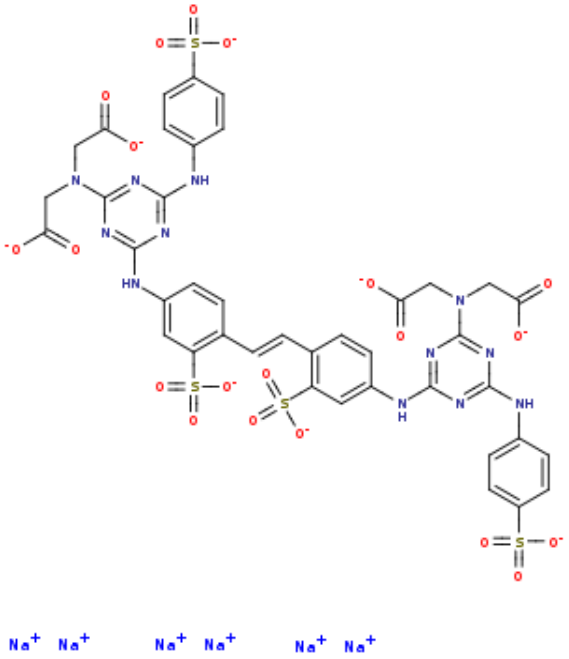
784157-49-9			EC number 424-260-3
778583-04-3			EC number 421-440-3

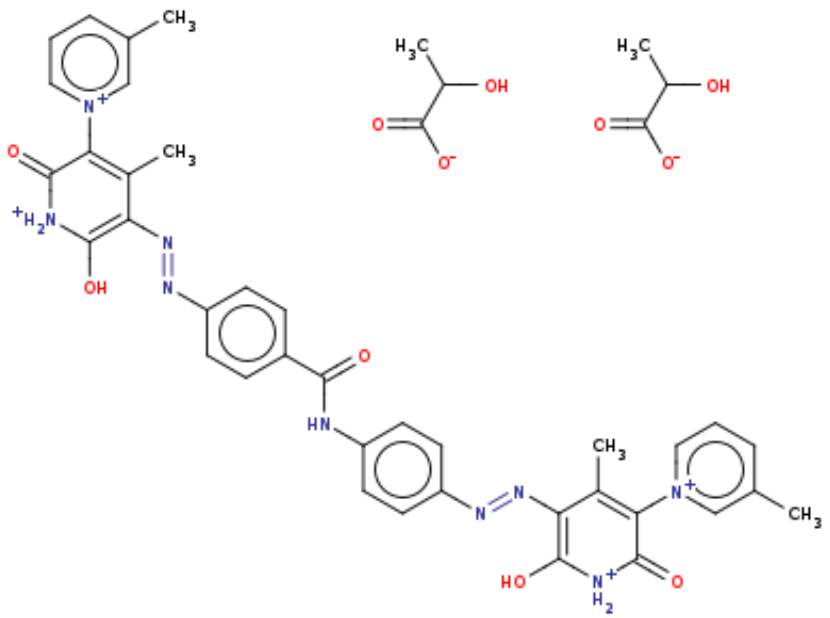
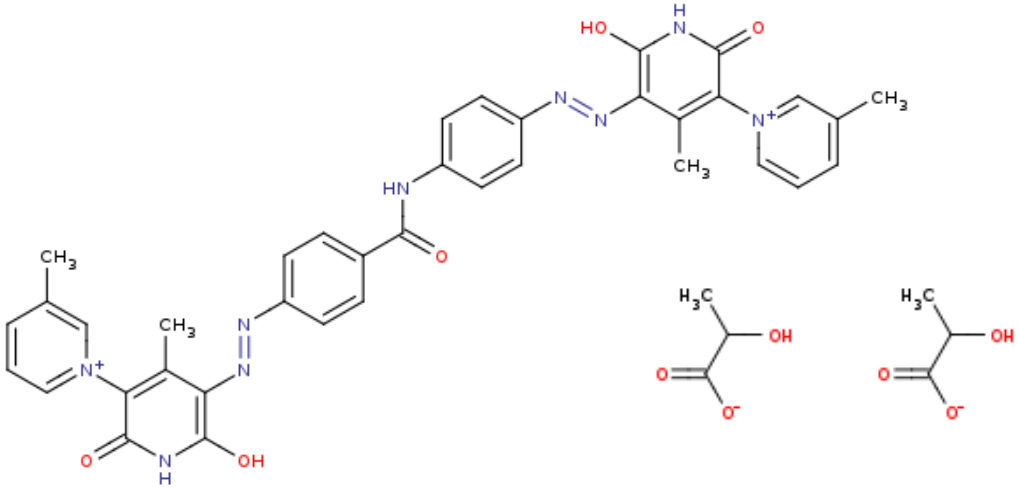
65-30-5			EC number 200-606-7
183487-56-1	HCl 		EC number 439-750-2 CAS RN™ is not with HCl
1265906-36-2			EC number 825-439-2

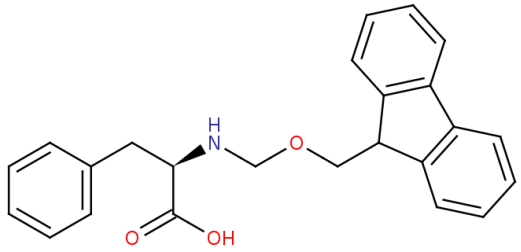
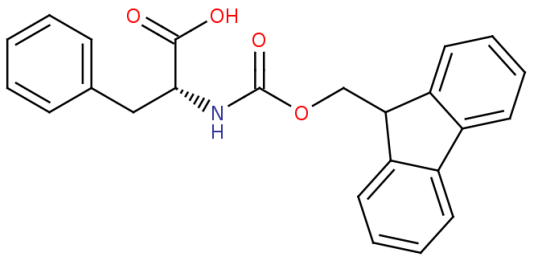
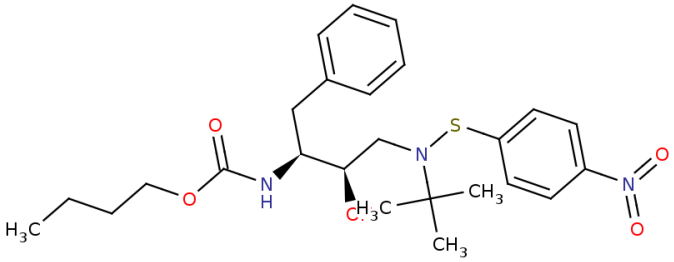
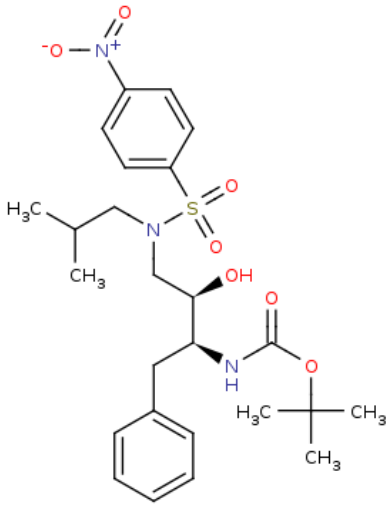
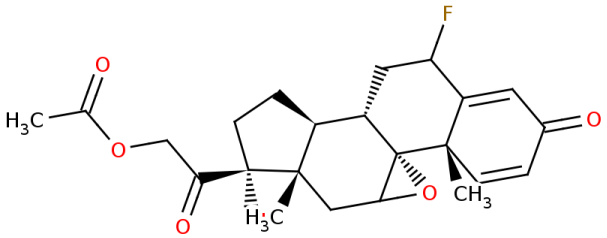
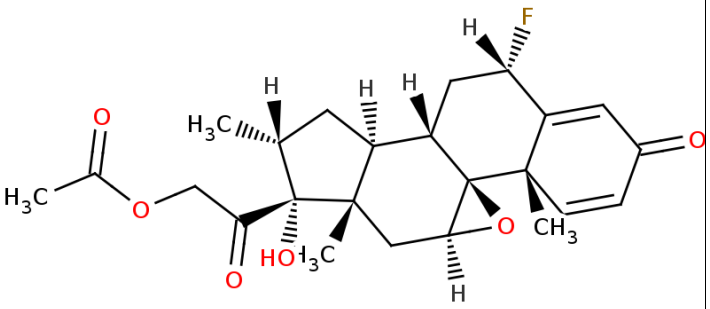
156137-33-6	 		EC number 423-520-3 CAS contains only the second structure
16881-77-9	 		EC number 240-914-9
2212-10-4			EC number 218-657-9

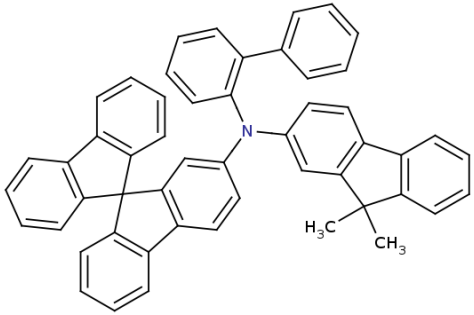
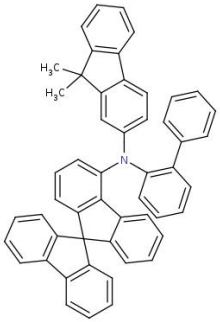
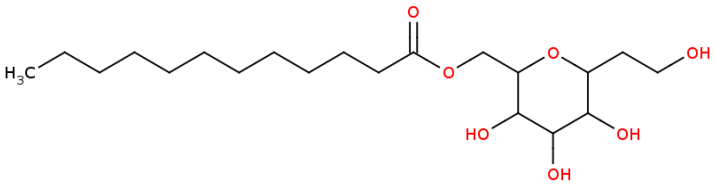
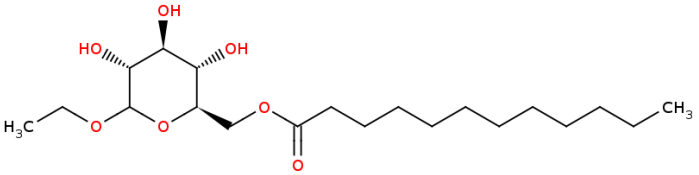
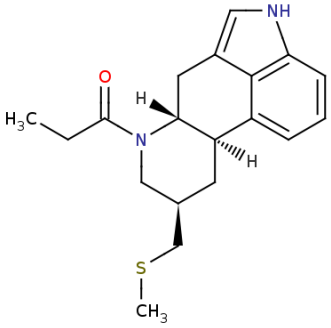
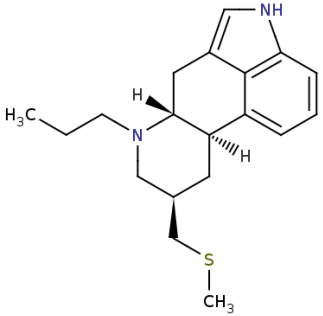
86168-95-8	 		EC number 401-300-8 CAS contains only the second structure

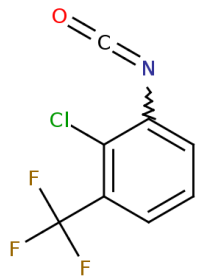
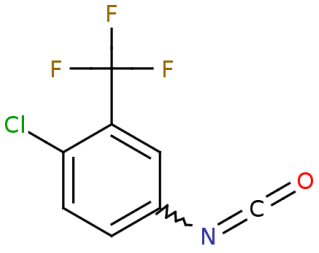
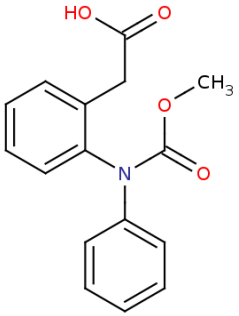
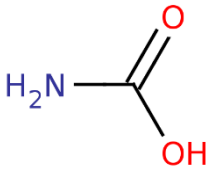
134127-48-3			EC number 420-680-6
97148-39-5			EC number 405-990-1 additional water that is not in the CAS registration
5324-84-5	 additional water that is not in the CAS registration		EC number 226-195-4

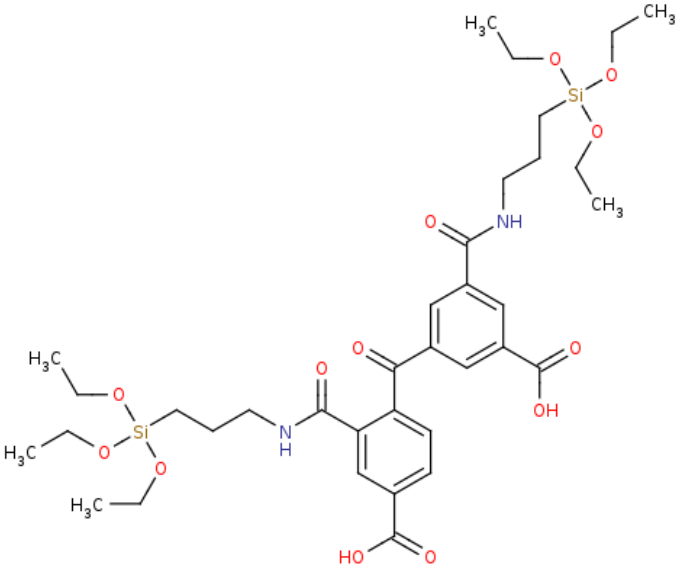
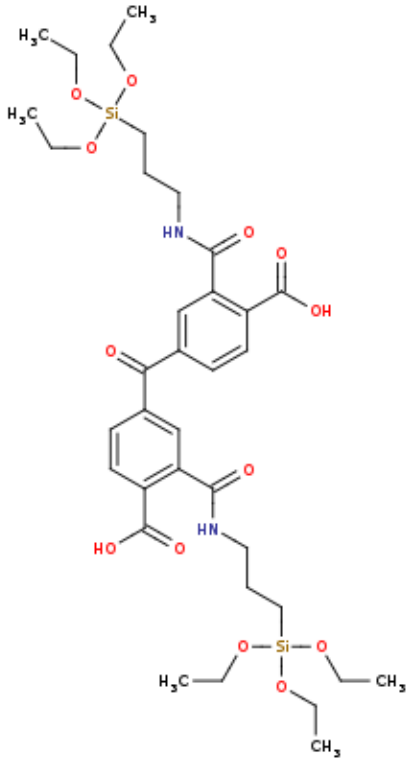
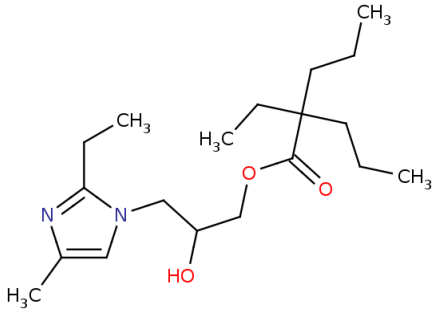
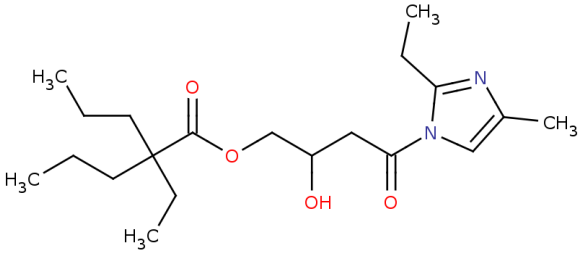
3734-33-6			EC number 223-095-2 additional water that is not in the CAS registration
174305-36-3			EC number 416-640-2 additional water that is not in the CAS registration

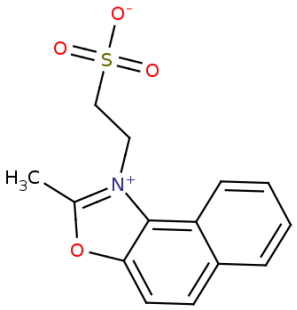
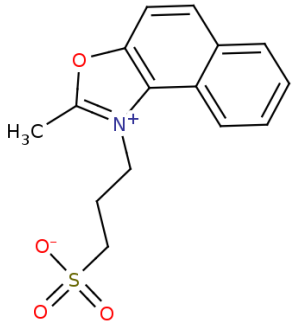
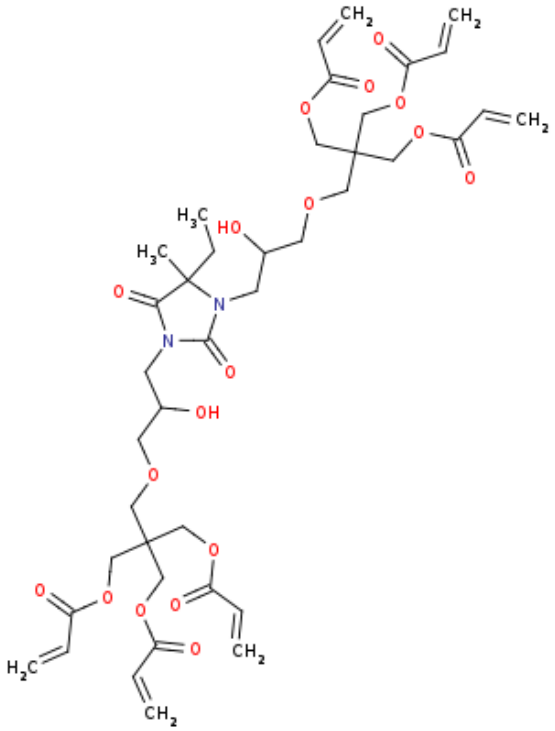
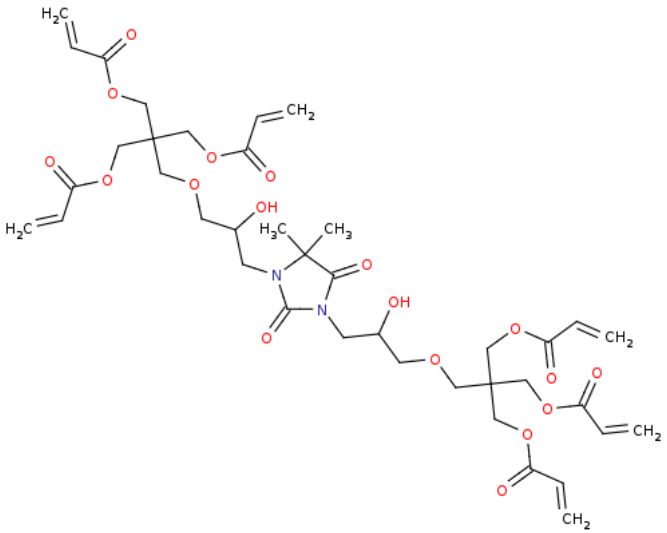
75214-63-0 (incorrect form)		EC number 278-130-4
75214-63-0 (correct form)		EC number 278-130-4

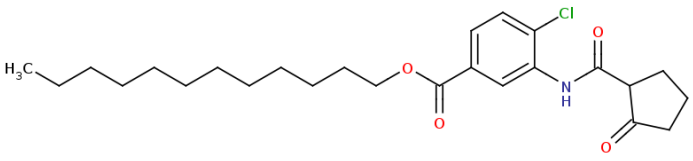
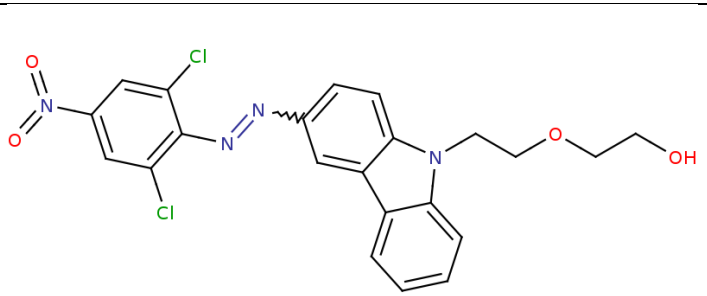
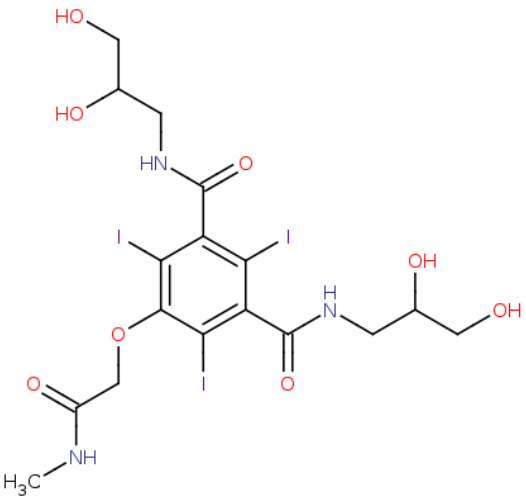
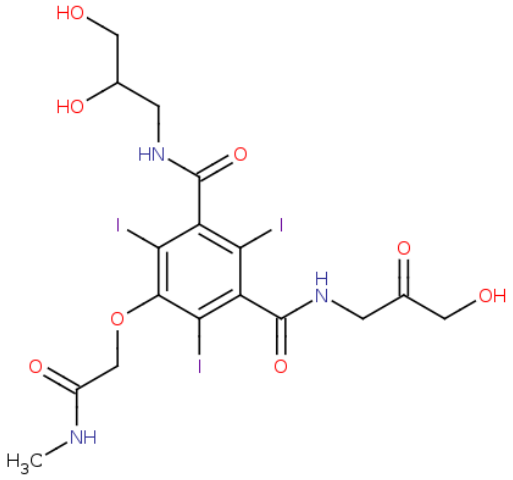
86123-10-6			EC number 440-090-2
191226-98-9			EC number 467-070-6
4571-51-1			EC number 941-489-9

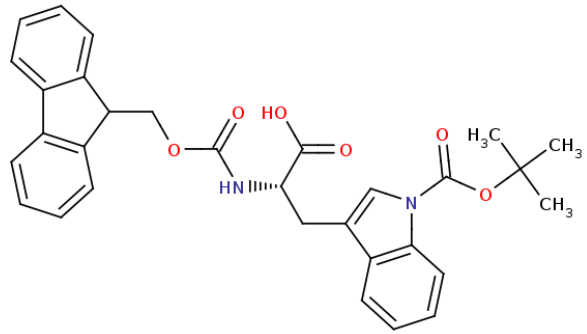
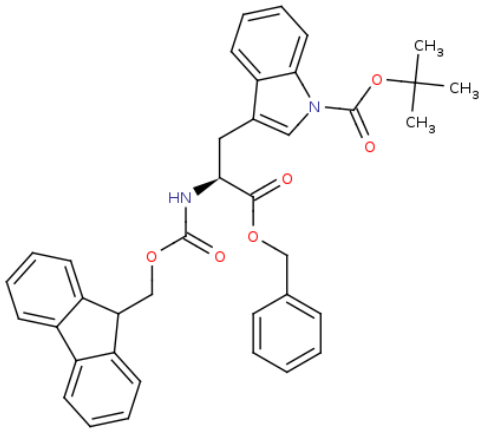
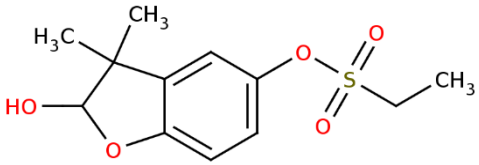
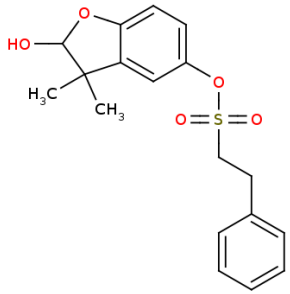
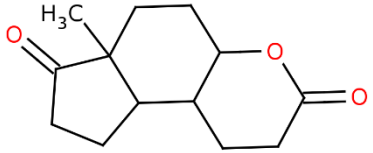
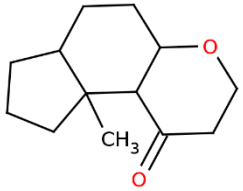
1450933-44-4			EC number 700-681-0
124285-43-4			EC number 418-610-4
66104-22-1			EC number 440-900-4

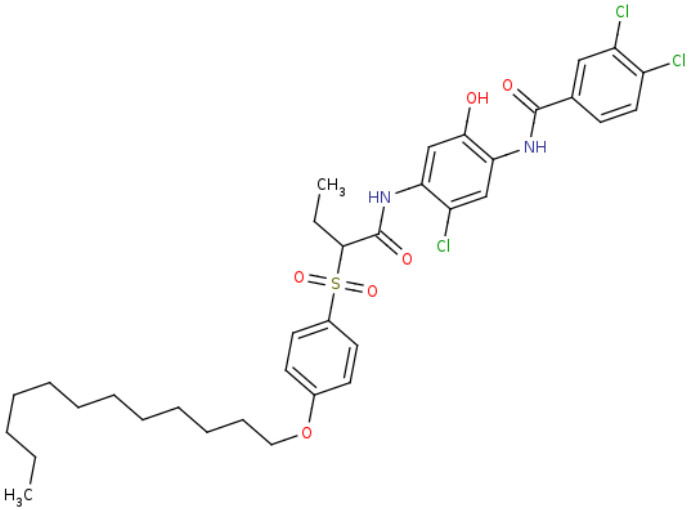
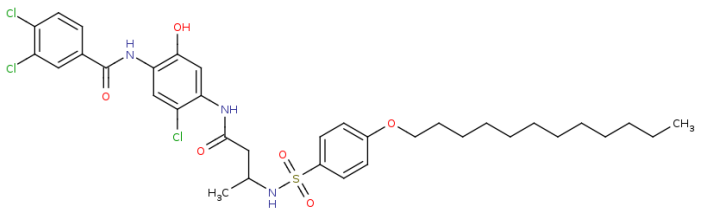
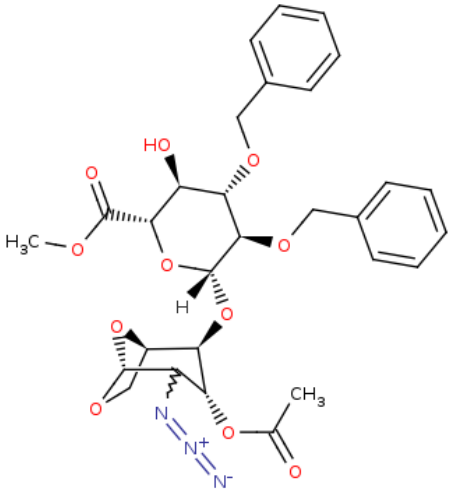
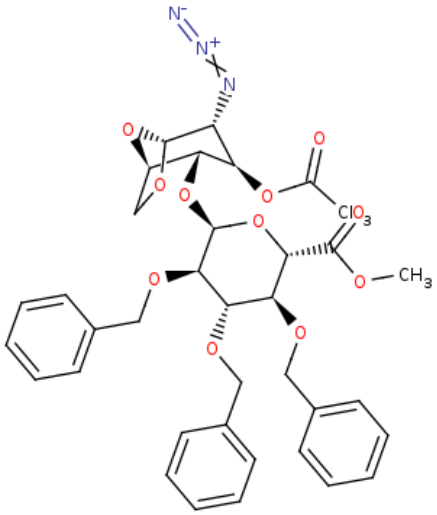
327-78-6			EC number 455-070-9
463-77-4			EC number 439-530-6

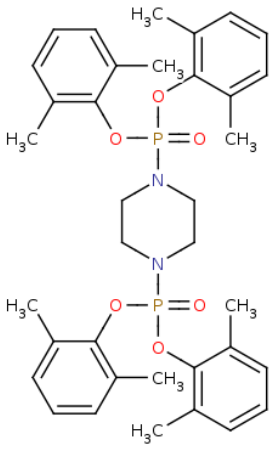
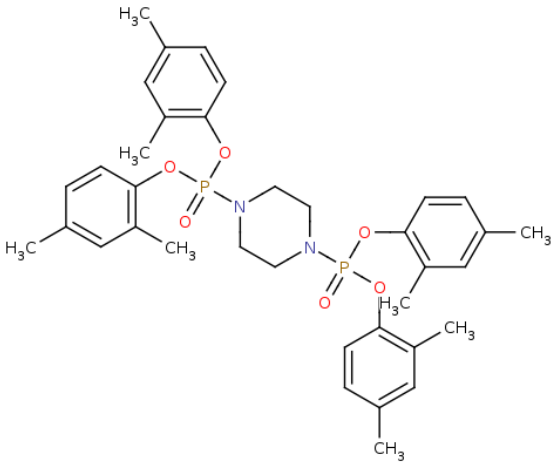
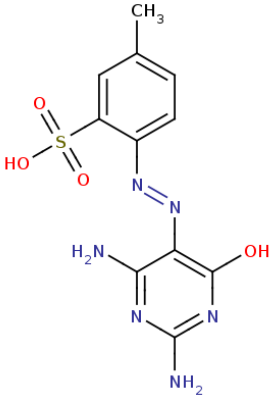
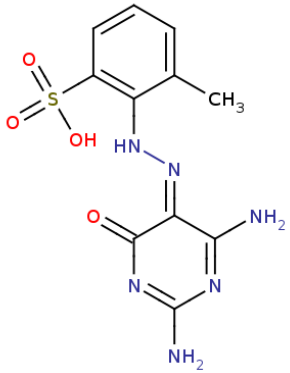
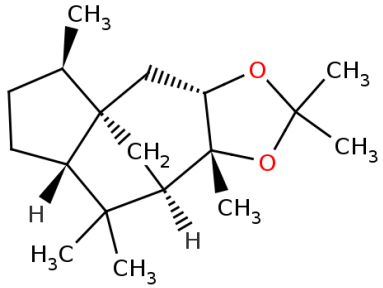
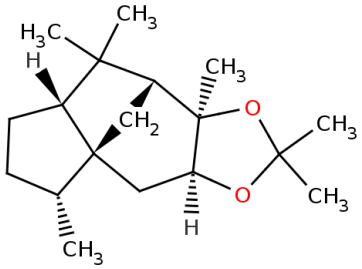
1010697-95-6			EC number 419-190-5
776326-15-9			EC number 417-350-9

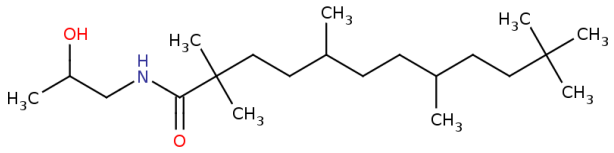
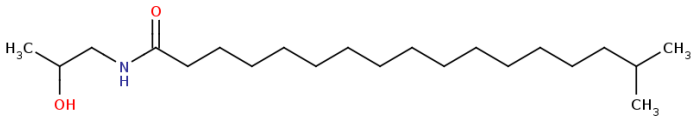
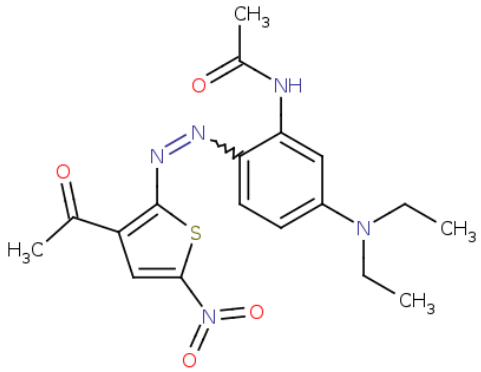
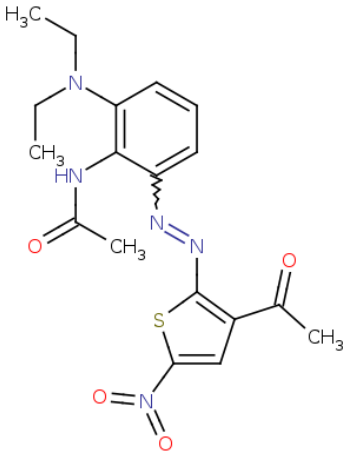
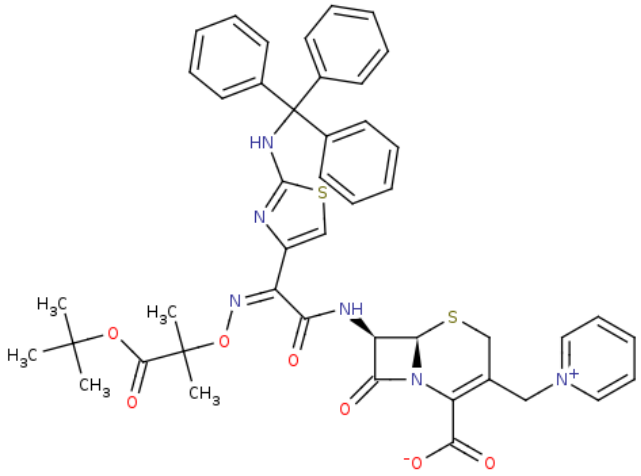
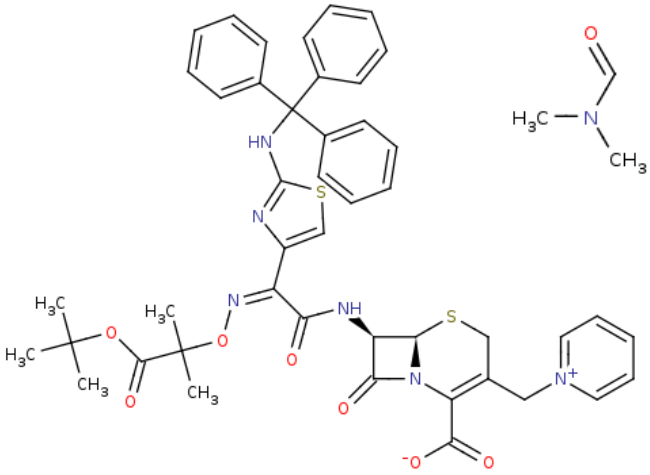
71806-08-1			EC number 421-030-4
79794-60-8			EC number 422-620-4

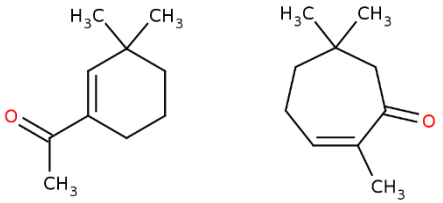
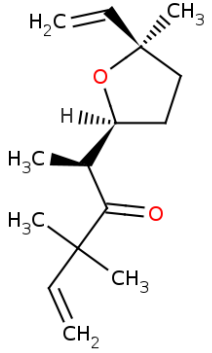
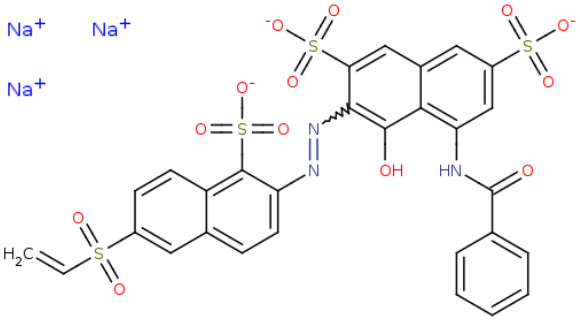
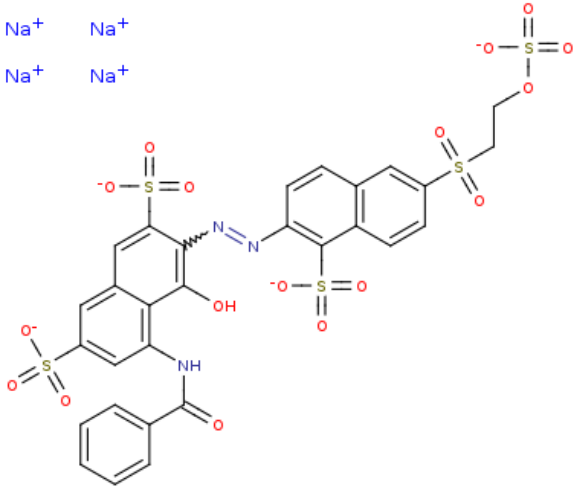
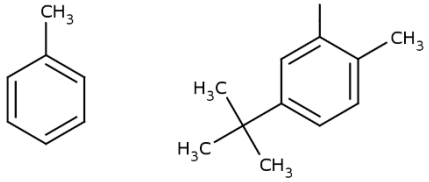
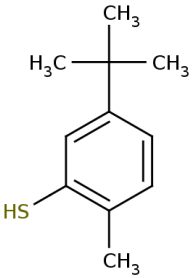
2135870-35-6			EC number 428-240-5
2135874-53-0			EC number 430-120-2

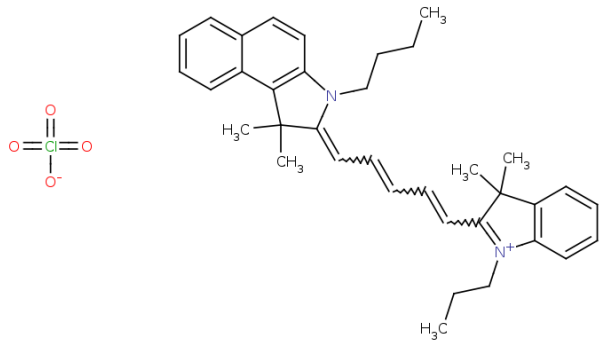
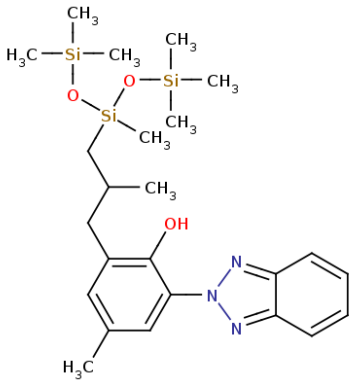
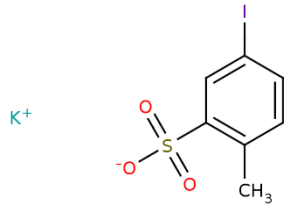
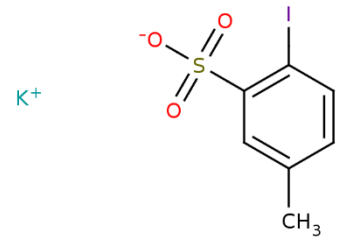
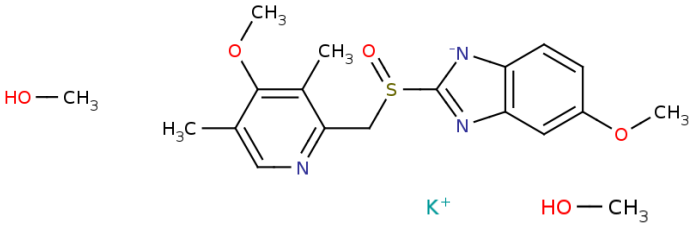
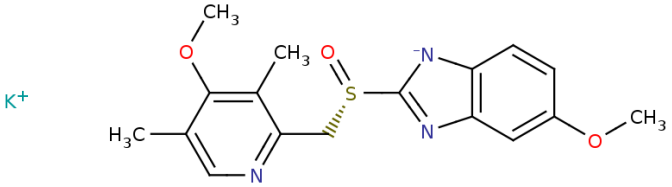
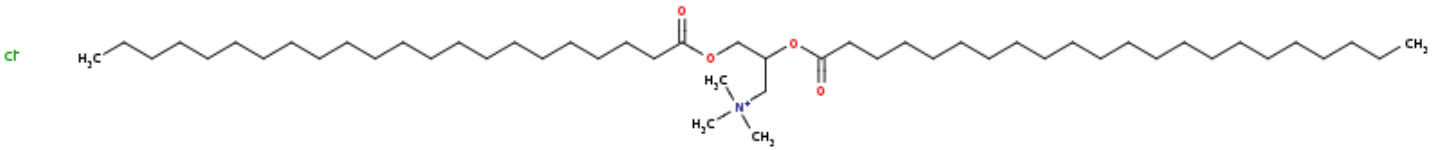
1170938-31-4			EC number 440-830-4
134144-37-9			EC number 402-720-4
148292-46-0			EC number 403-860-9

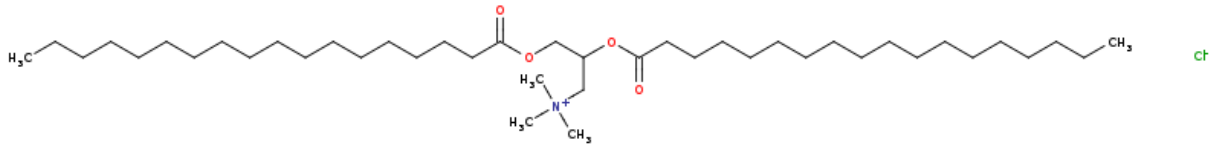
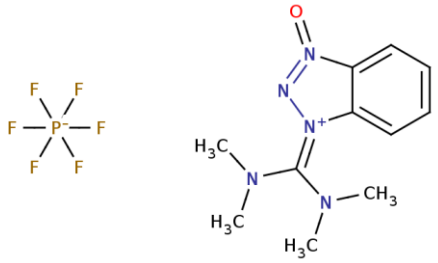
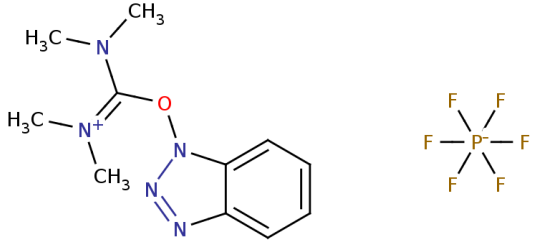
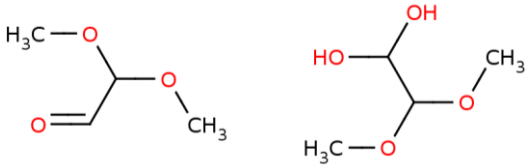
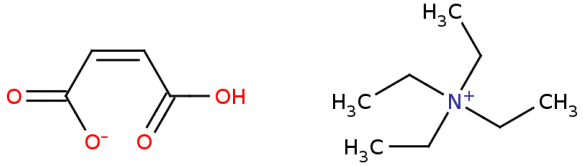
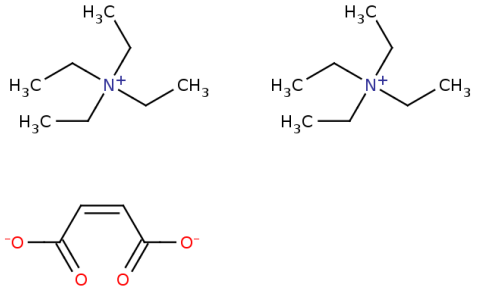
327092-50-2			EC number 431-130-1
115195-66-9			EC number 433-070-1

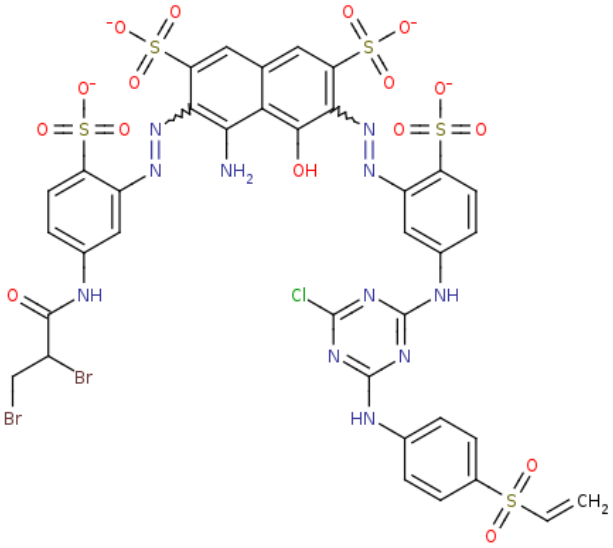
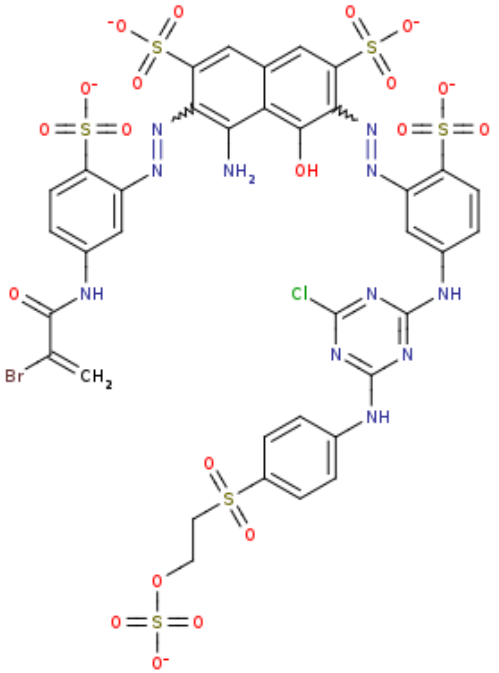
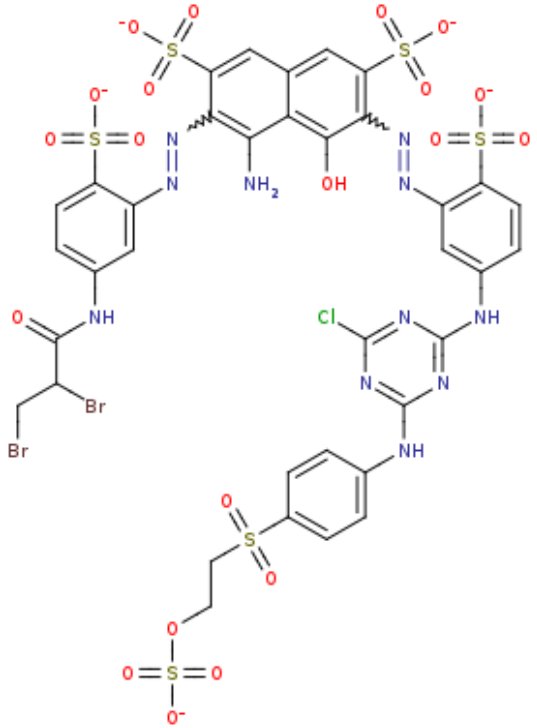
382138-32-1			EC number 433-550-9
1333483-07-0			EC number 700-002-8
2135337-60-7			EC number 427-580-1

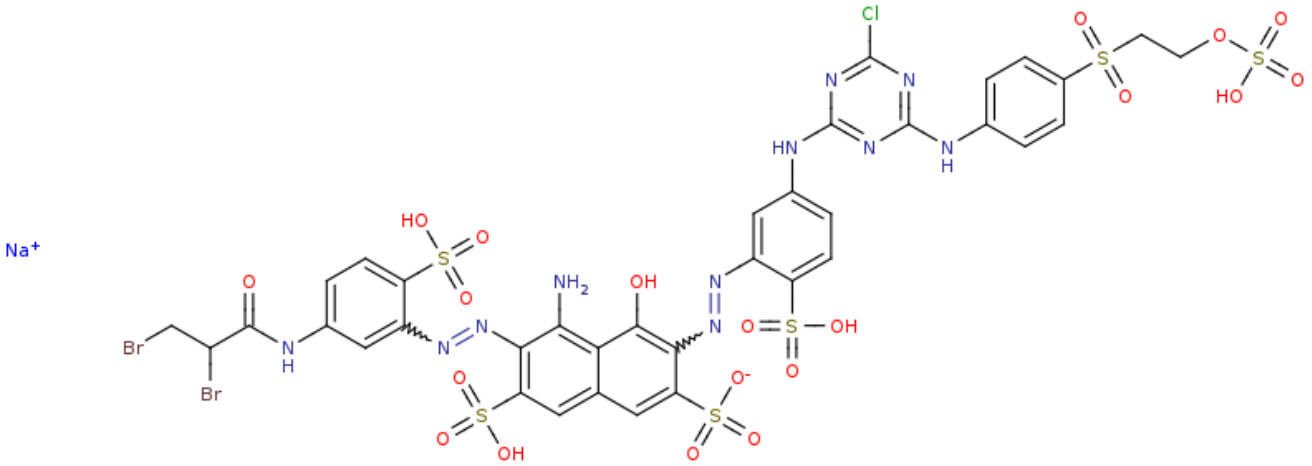
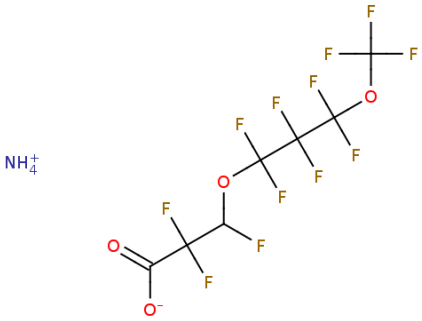
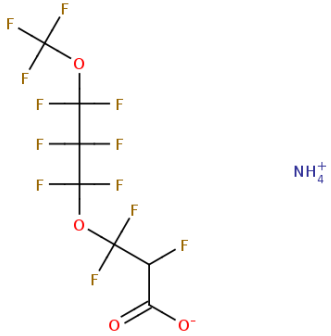
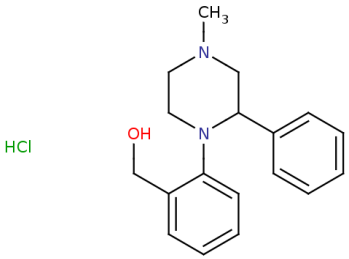
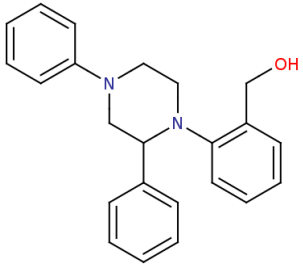
170573-32-7			EC number 431-540-9
777891-21-1			EC number 416-860-9
84377-83-3			EC number 617-560-2

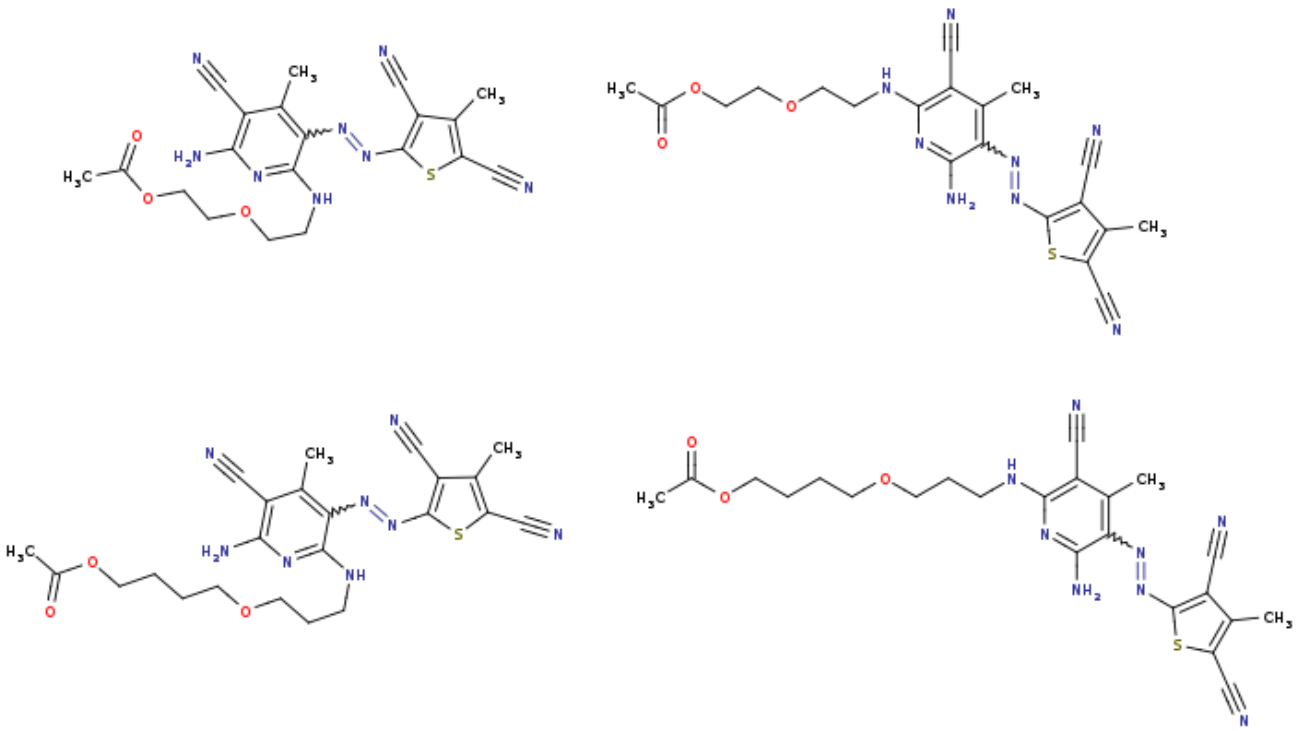
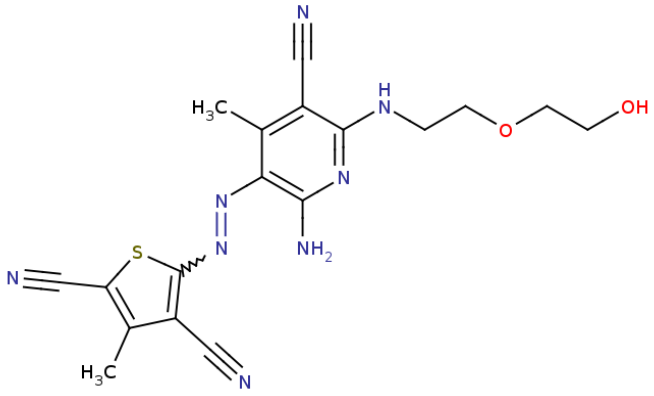
30925-48-5			EC number 415-570-1
98114-32-0			EC number 423-200-3
7340-90-1			EC number 444-970-7

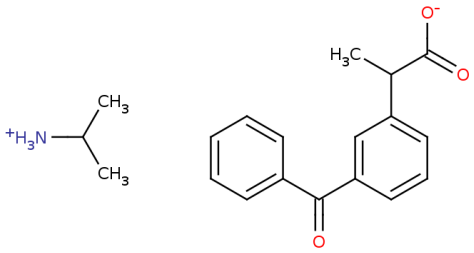
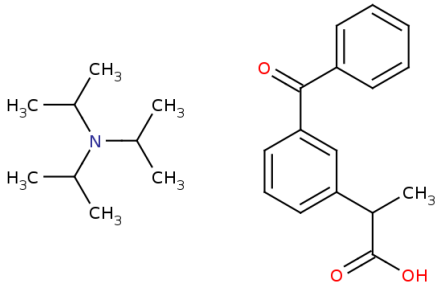
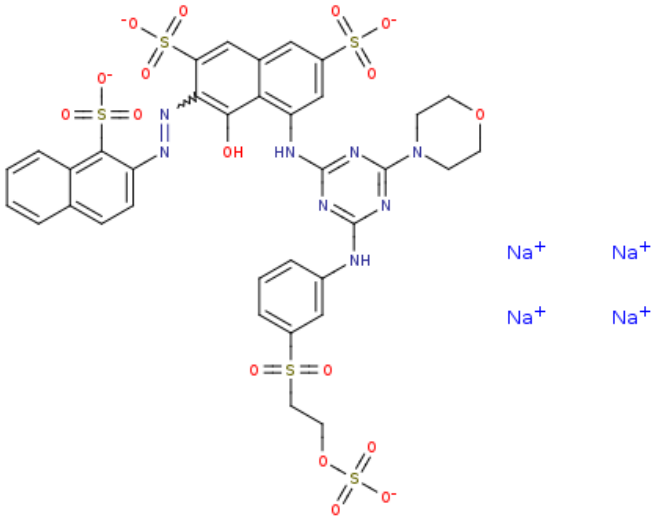
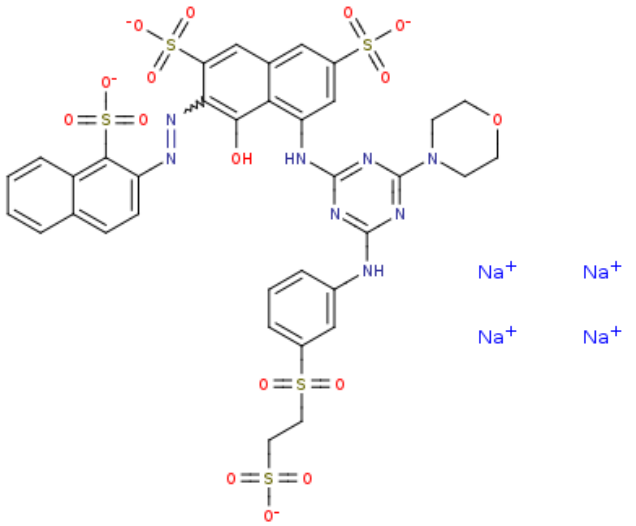
155633-54-8			EC number 423-660-5
1093215-92-9			EC number 426-300-5
161796-84-5			EC number 449-880-1
220609-41-6 (incorrect form)			EC number 405-660-7

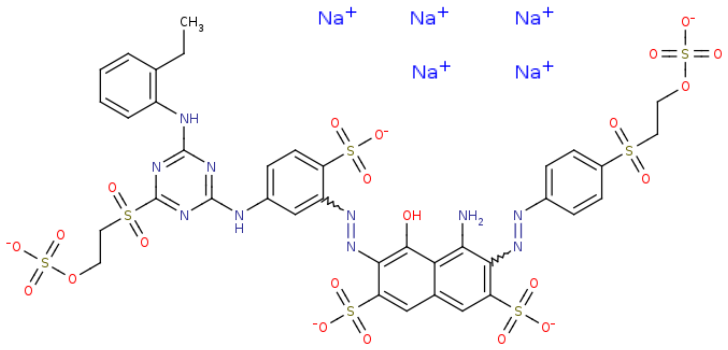
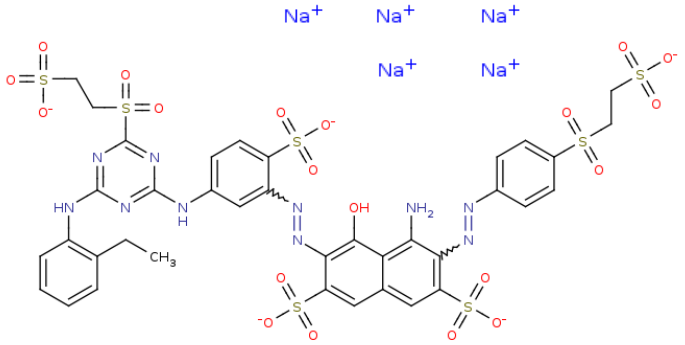
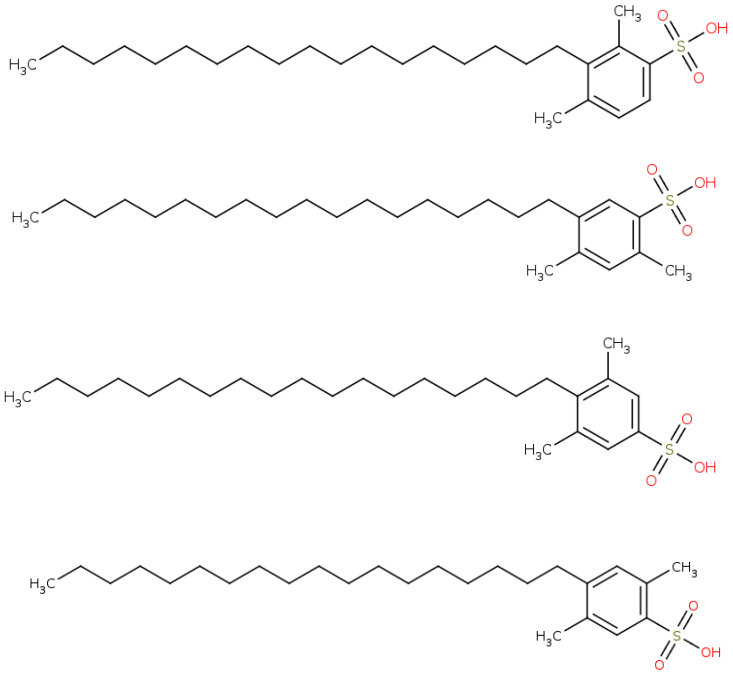
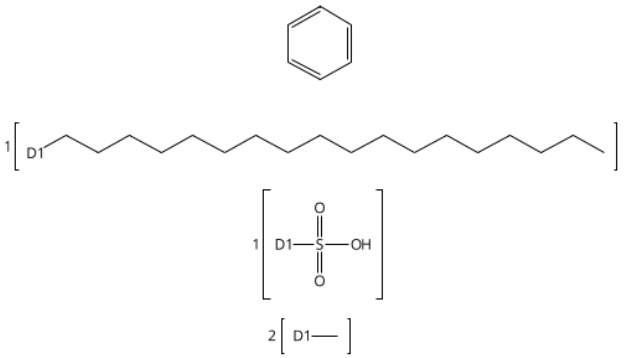
220609-41-6 (correct form)		EC number 405-660-7
625384-22-7	 	EC number 423-020-5
51673-84-8		EC number 421-890-0
111754-40-6	 	EC number 457-950-8

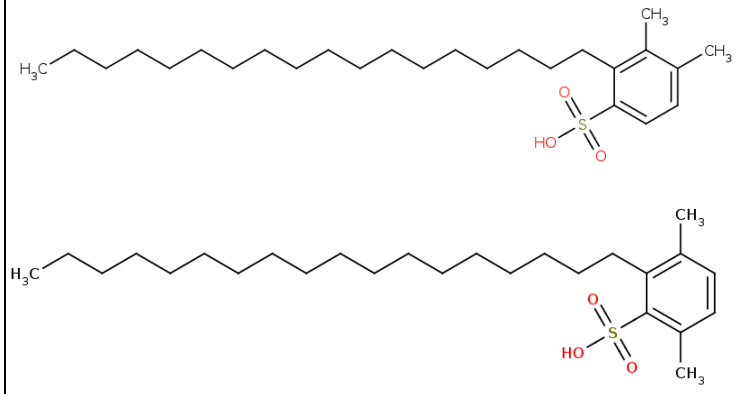
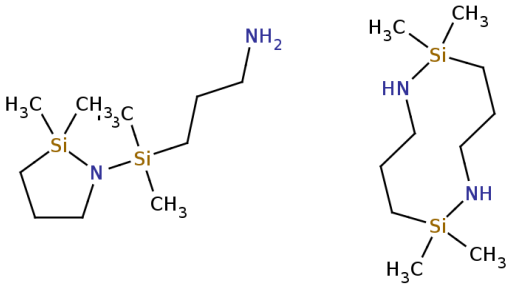
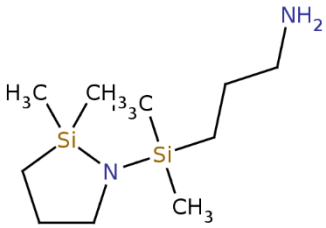
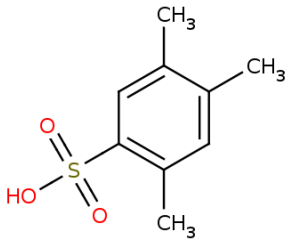
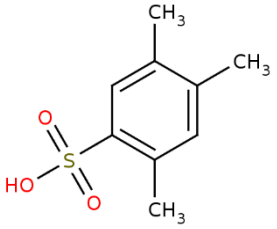
180778-23-8 (incorrect form)	   Na^+ Na^+ Na^+ Na^+ Na^+ Na^+ Na^+ Na^+ Na^+ Na^+ Na^+ Na^+	EC number 424-320-9

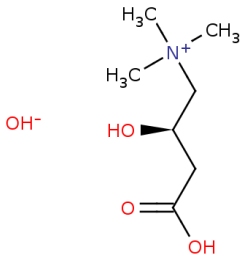
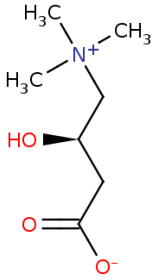
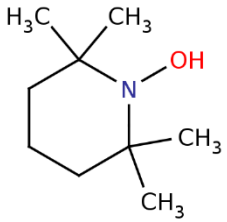
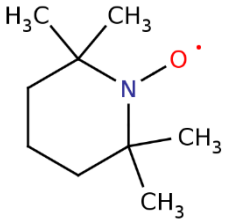
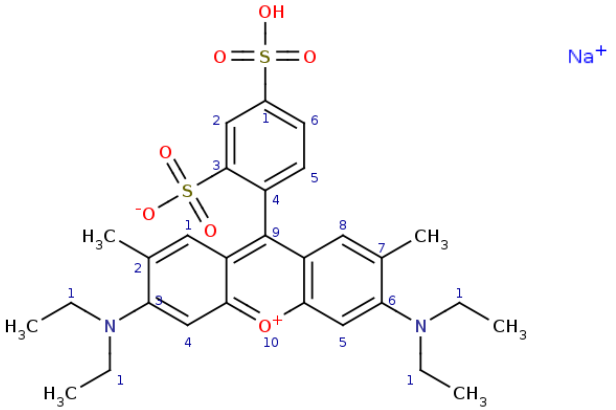
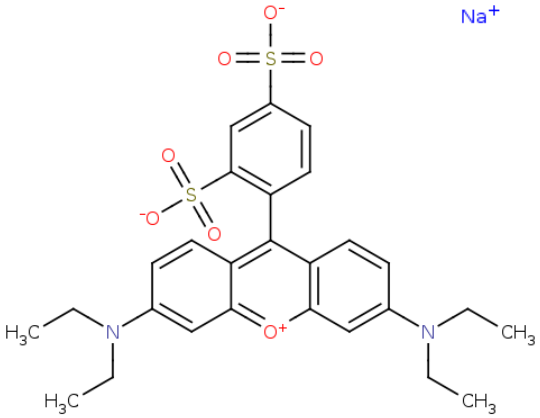
180778-23-8 (correct form)			
1280222-90-3			EC number 480-310-4
1379676-70-6			EC number 420-200-5

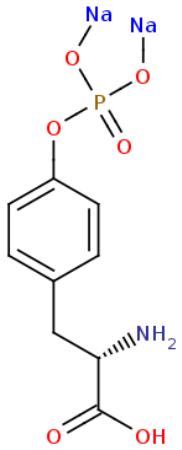
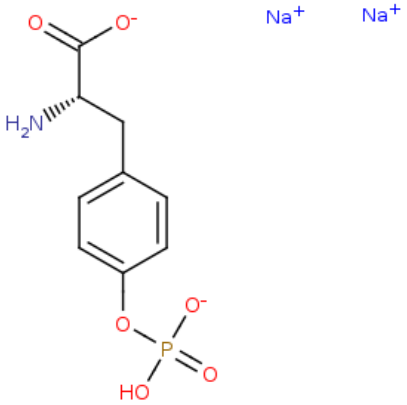
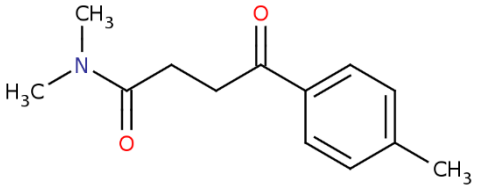
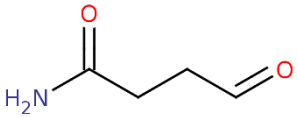
107815-88-3 (incorrect form)		EC number 410-530-8
107815-88-3 (correct form)		EC number 410-530-8

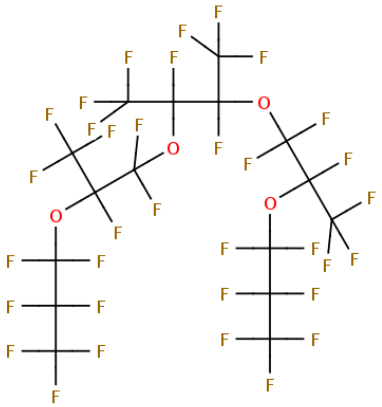
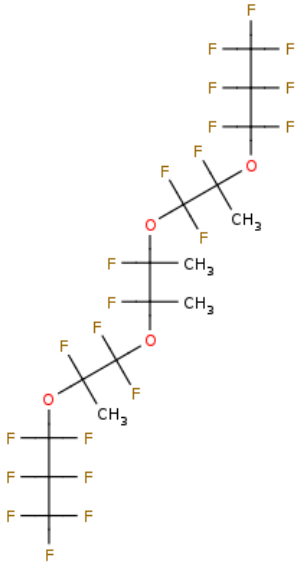
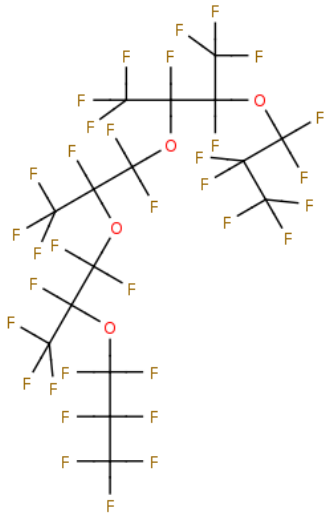
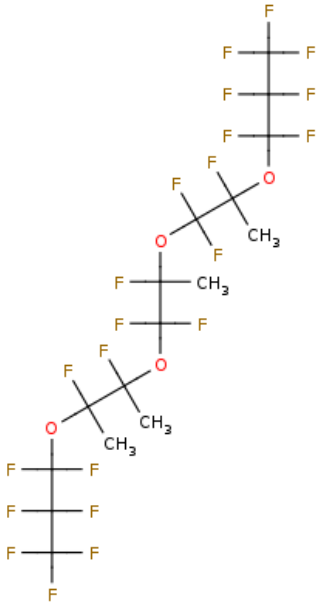
1379932-74-7			EC number 417-970-1
1379676-82-0			EC number 413-070-6

1379676-74-0			EC number 423-790-2
148262-93-5		 • 1/2 Ca Ca should also be Ca^{2+} and SO_3H should be SO_3^-	EC number 402-040-8

			
388606-32-4			EC number 470-090-8
3453-84-7			EC number 420-770-5

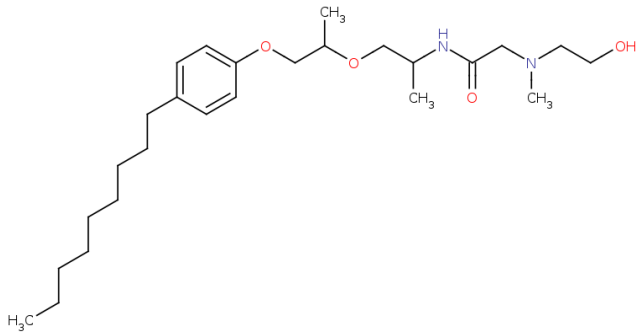
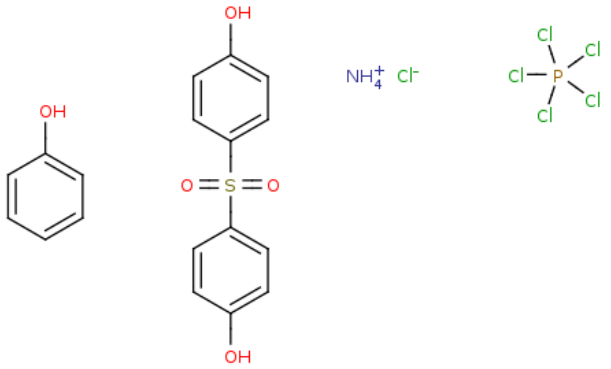
541-15-1			EC number 208-768-0
2564-83-2			EC number 219-888-8
3520-42-1			EC number 222-529-8

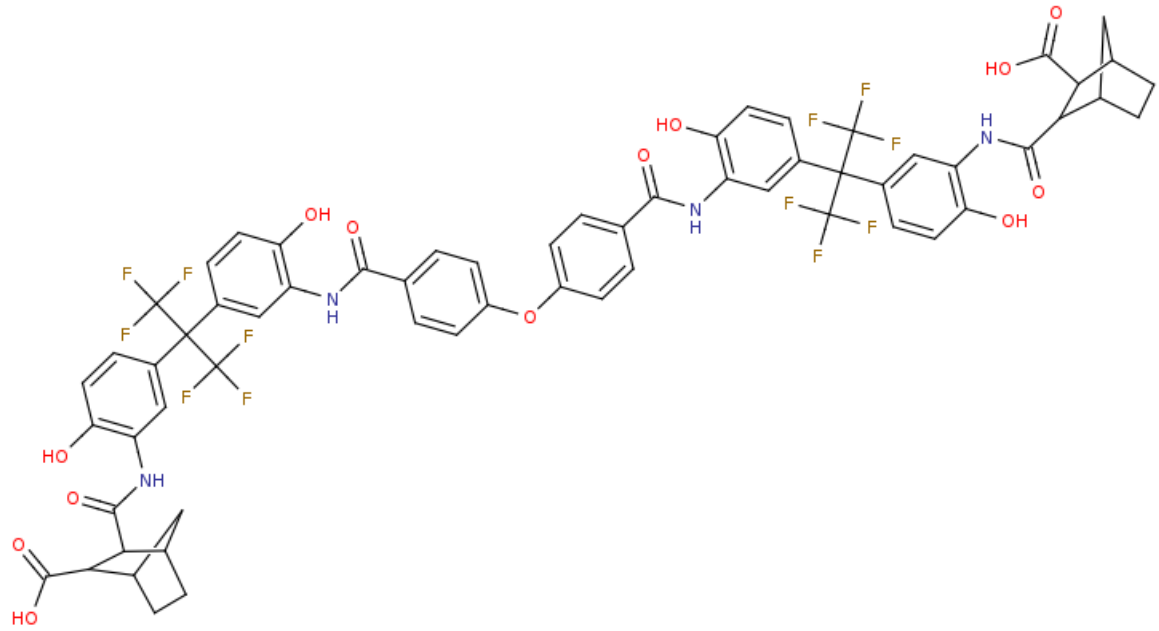
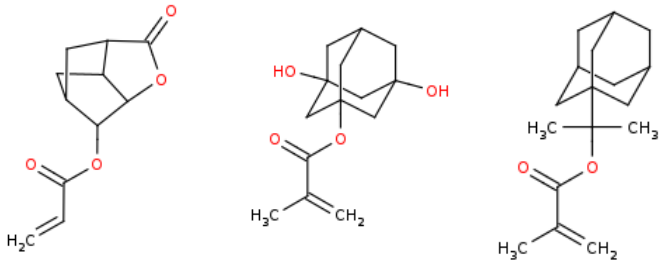
1610350-91-8			EC number 860-352-3
27719-81-9			EC number 464-950-1

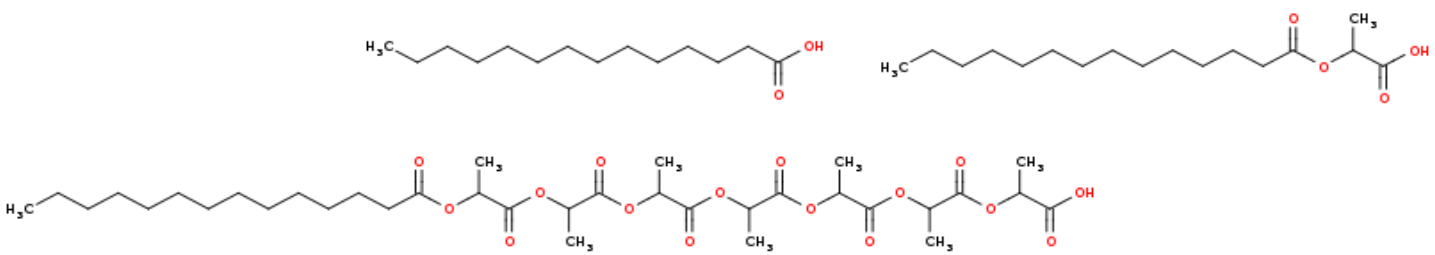
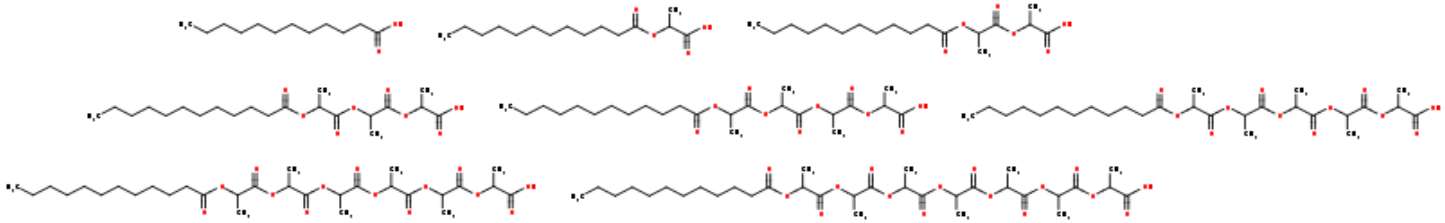
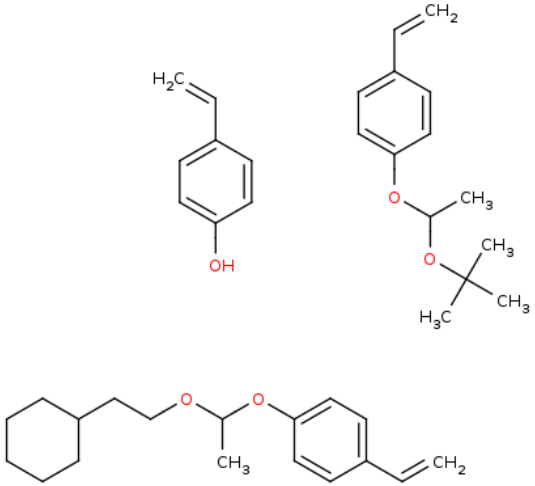
148292-43-7			EC number 404-710-5
148292-47-1			EC number 404-730-4

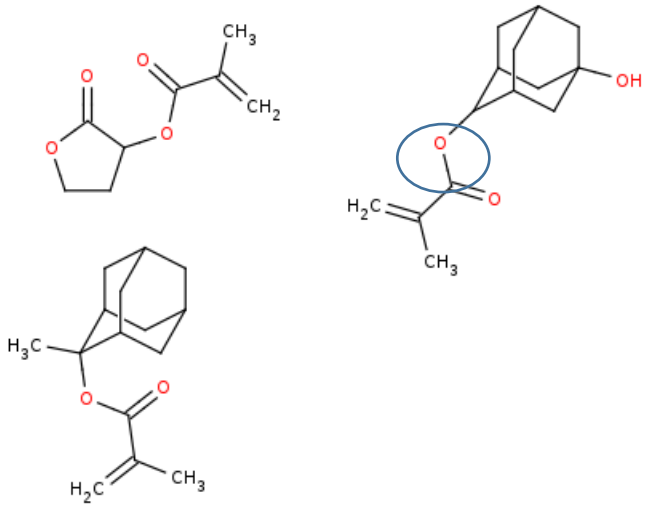
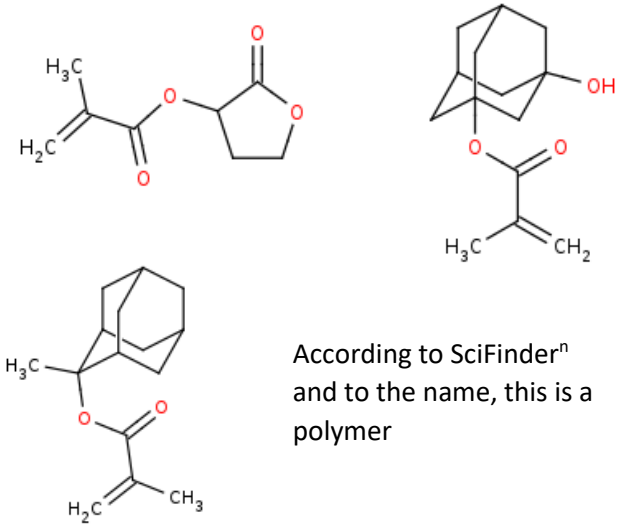
2) Monomer shown for a polymer

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

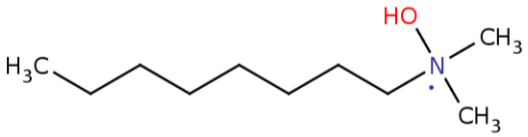
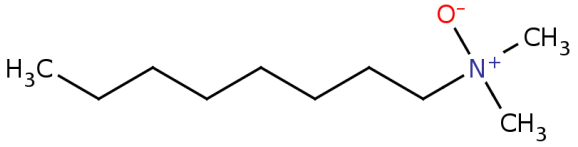
-	 According to the name, this is a polymer (POLYAMIDE RESIN)		EC number 426-580-9
-		According to the name, this is a polymer (2-Propenoic acid, 2-methyl-, 3,5-dihydroxytricyclo[3.3.1.13,7]dec-1-yl ester, polymer with hexahydro-2-oxo-3,5-methano-2H-cyclopenta[b]furan-6-yl 2-propenoate and 1-methyl-1-tricyclo[3.3.1.13,7]dec-1-ylethyl-2-methyl-2-propenoate)	EC number 473-380-2

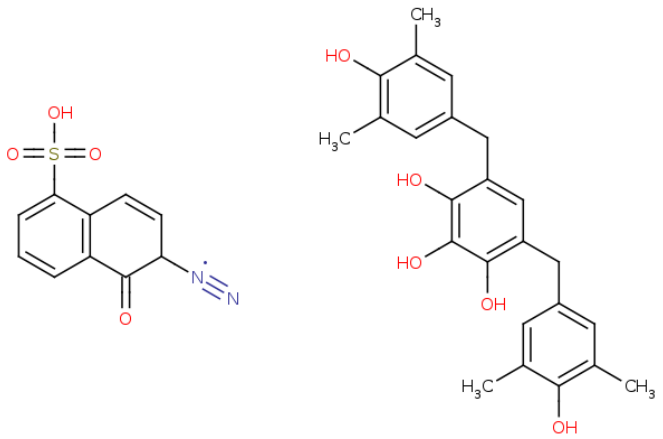
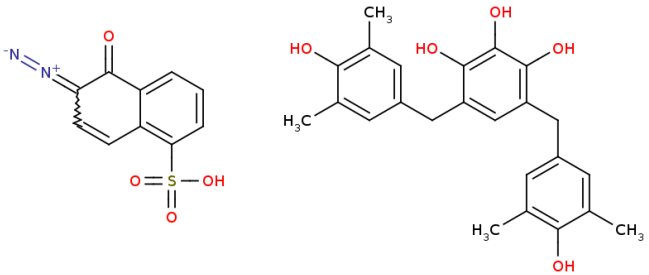
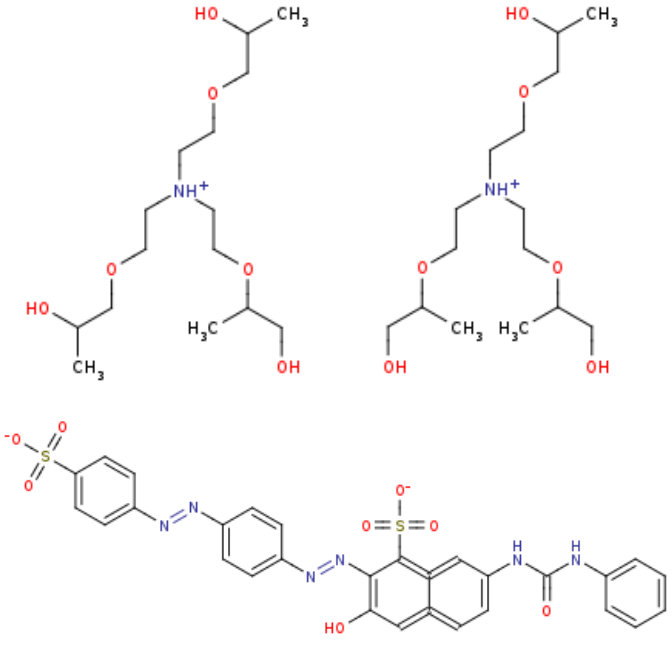
174591-51-6	 According to SciFinder^{n} and to the name, this is a polymer.		EC number 412-580-6
58856-63-6	 According to SciFinder^{n} and to the name, this is a polymer.		EC number 412-590-0
-		According to the name, this is a polymer (Phenol, 4-ethenyl-, homopolymer, 1-(2-cyclohexylethoxy)ethyl ethers)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

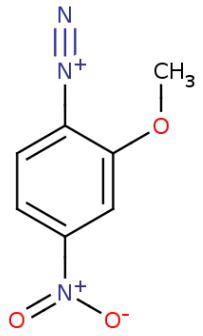
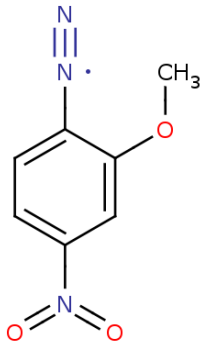
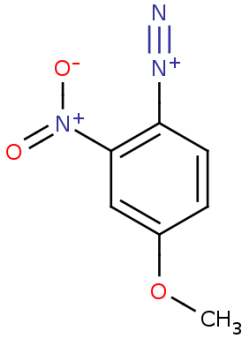
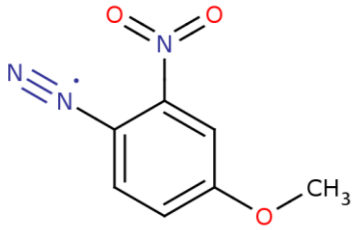
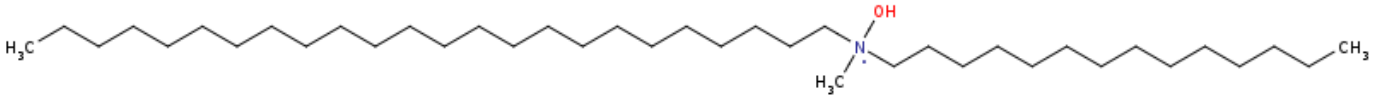
258879-87-7		 According to SciFinder^{n} and to the name, this is a polymer	EC number 442-950-2

3) Unusual valence

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

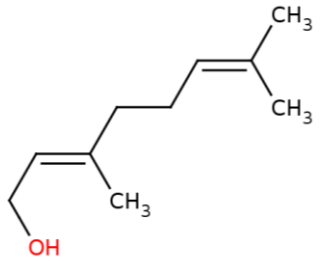
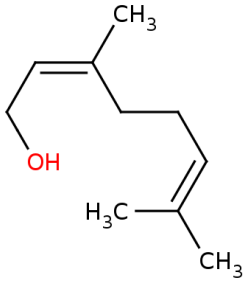
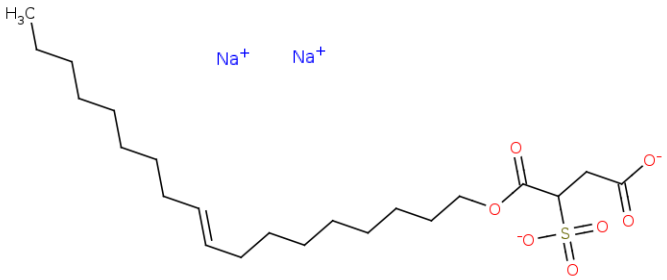
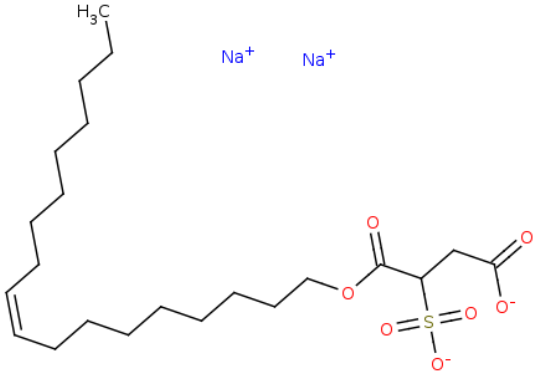
CAS RN™	Structure in the database	Structure corresponding to the CAS RN™	Comment
2605-78-9			EC number 607-854-9

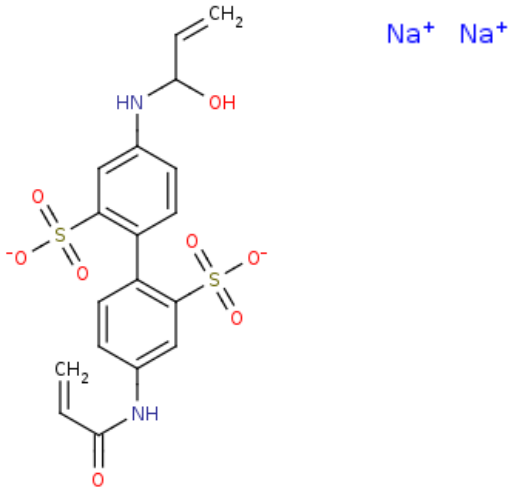
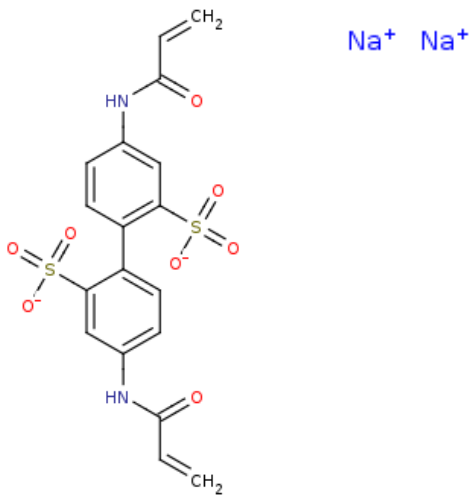
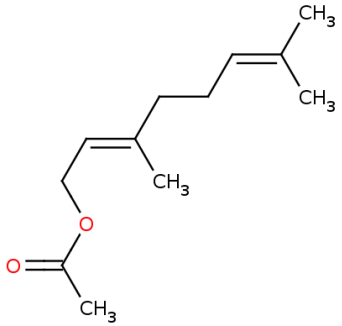
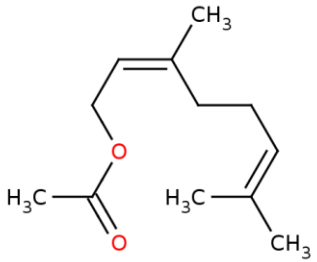
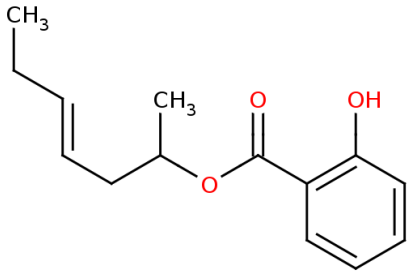
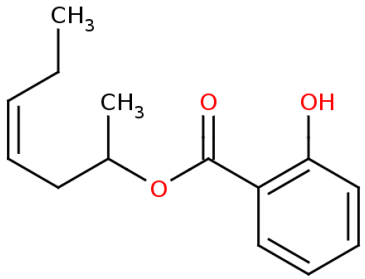
133686-87-0			EC number 451-140-8
1628433-99-7		Carbon should only have 4 bonds and not 5. Correct strucutre is not available elsewhere	EC number 406-170-6

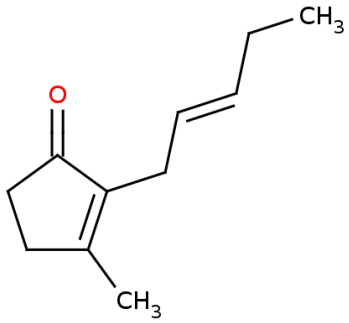
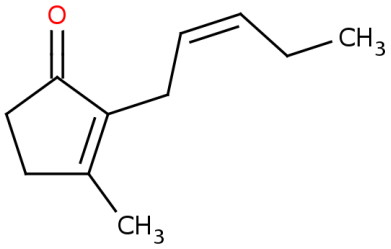
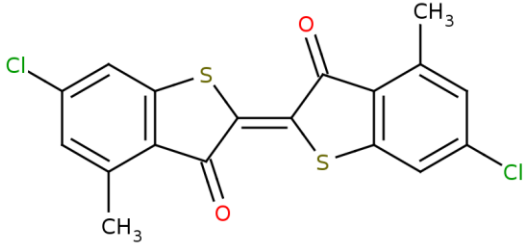
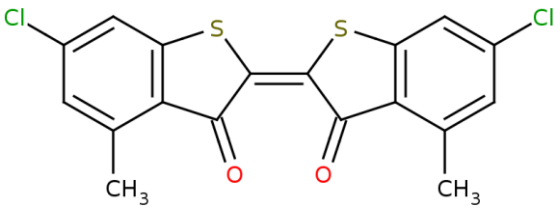
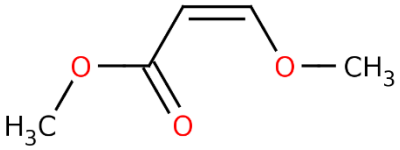
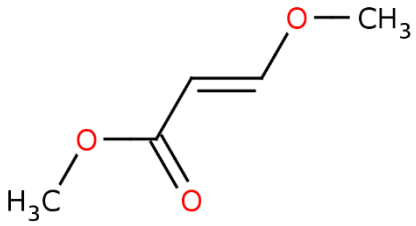
27761-26-8			EC number 248-642-2
27165-25-9			EC number 248-284-7
- (incorrect form)			EC number 440-250-1
- (correct form)	Substance could not be indentified in any of the other databases		EC number 440-250-1

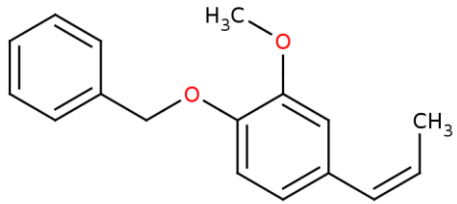
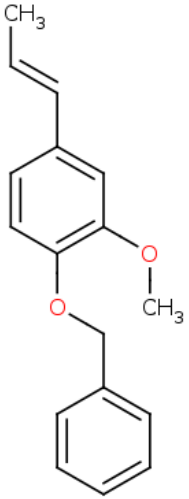
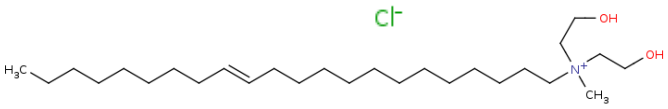
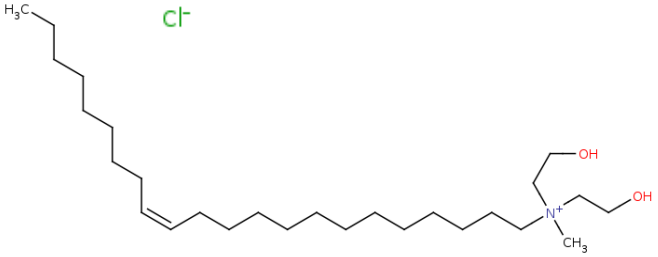
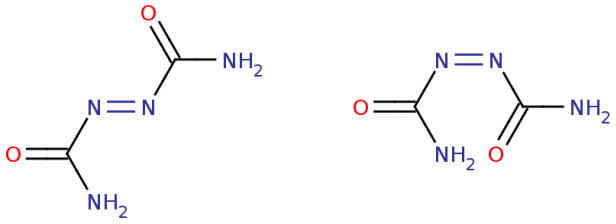
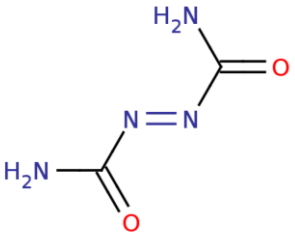
4) Inconsistency related to cis/trans isomers

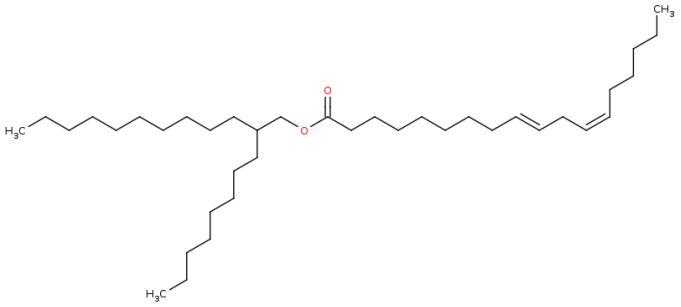
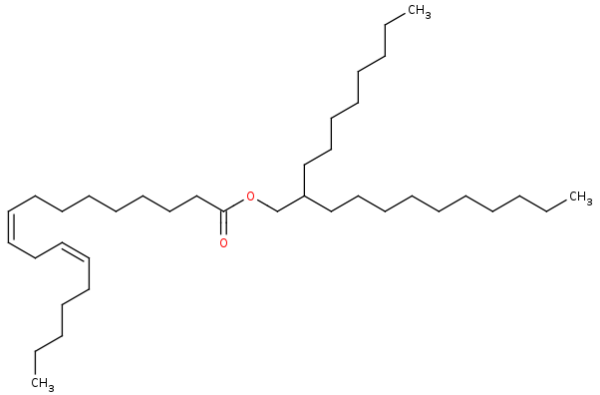
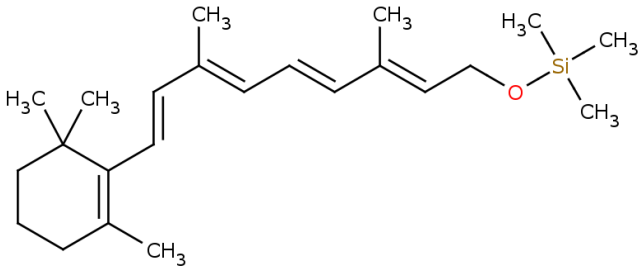
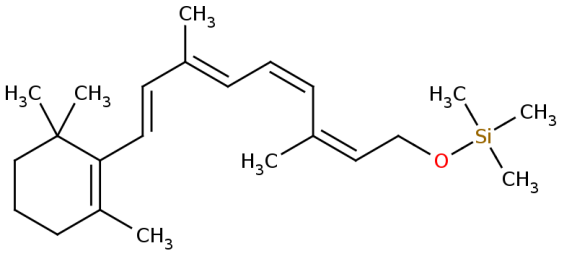
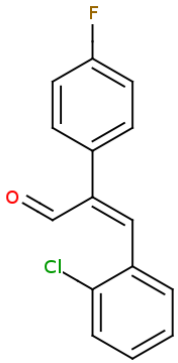
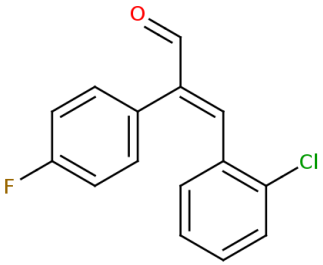
Table 4: Substances in the ECHA database where the SMILES do not correspond to the CAS RN™ as allocated in SciFinder^n. The reason for the mismatches here are deviations in the cis/trans isomers.

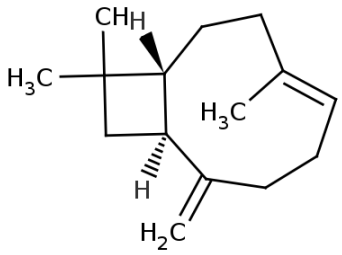
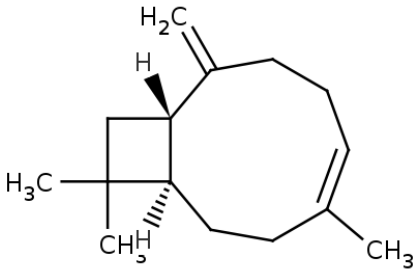
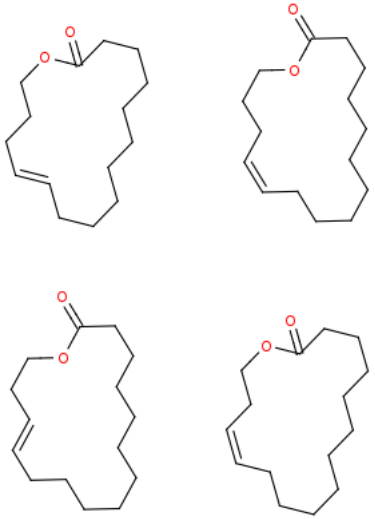
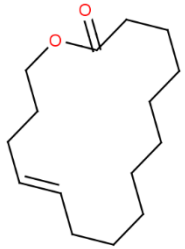
CAS RN™	Structure in the database	Structure corresponding to the CAS RN™	Comment
106-25-2			EC number 203-378-7
94213-67-9			EC number 303-773-5

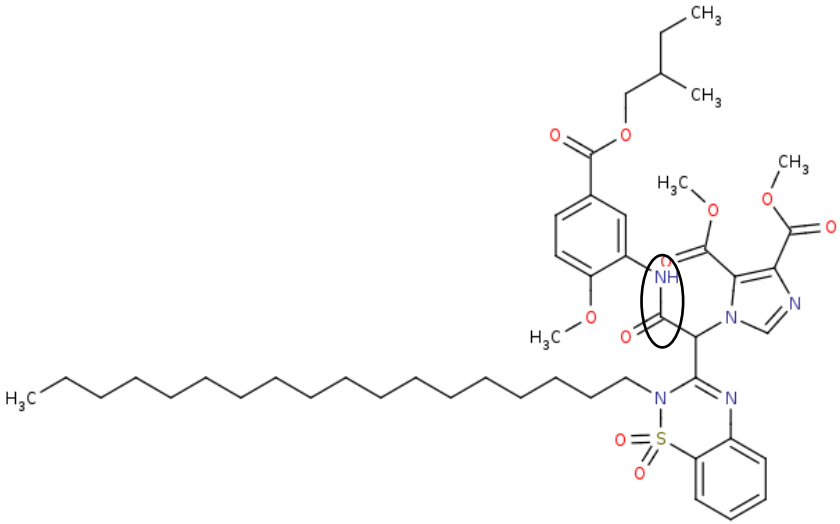
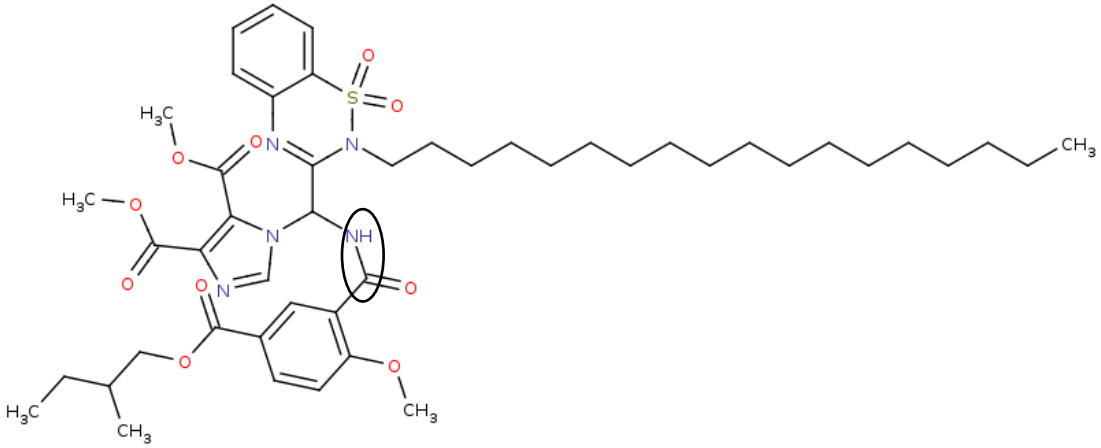
881539-89-5			EC number 812-549-0
141-12-8			EC number 205-459-2
873888-84-7			EC number 700-488-1

488-10-8			EC number 207-668-4
2379-74-0			EC number 219-163-6
5788-17-0			EC number 412-900-4

120-11-6			EC number 204-370-6
120086-58-0			EC number 426-210-6
123-77-3			EC number 204-650-8 CAS RN™ does not cover both forms

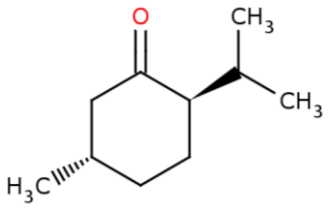
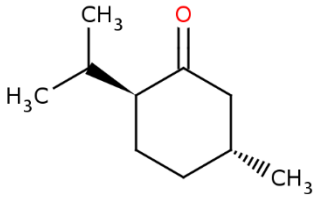
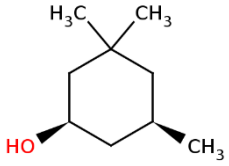
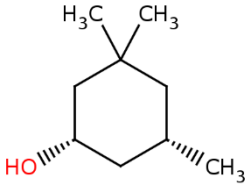
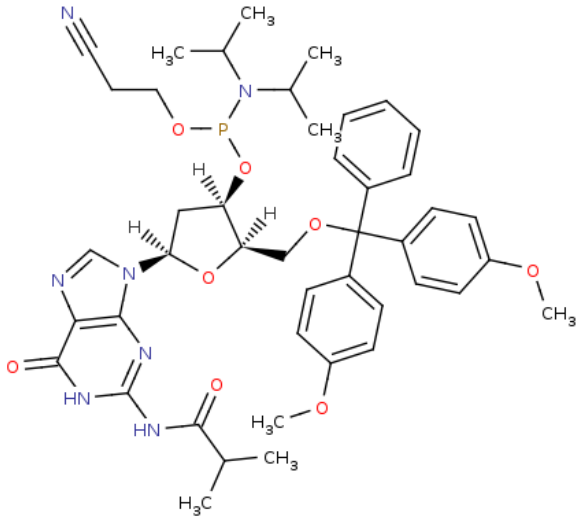
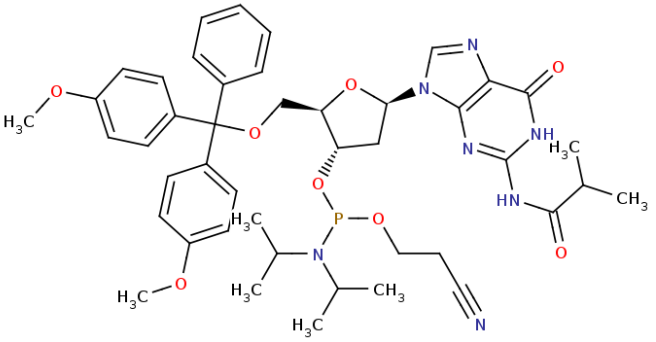
129423-60-5			EC number 438-100-5
16729-19-4			EC number 435-930-1
112704-51-5			EC number 410-980-5

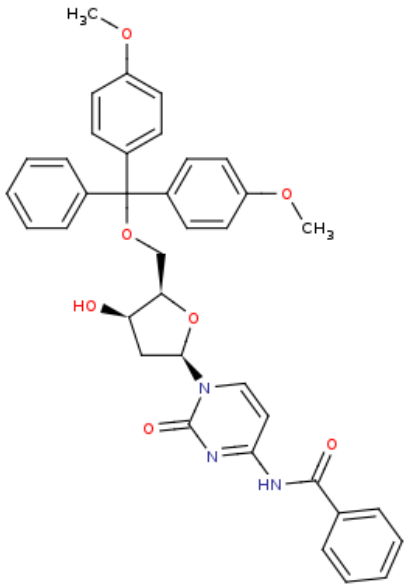
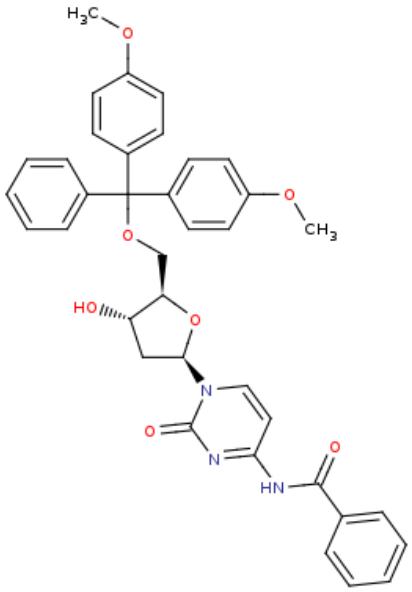
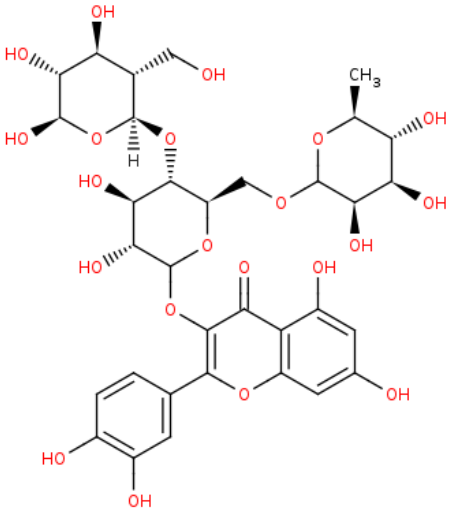
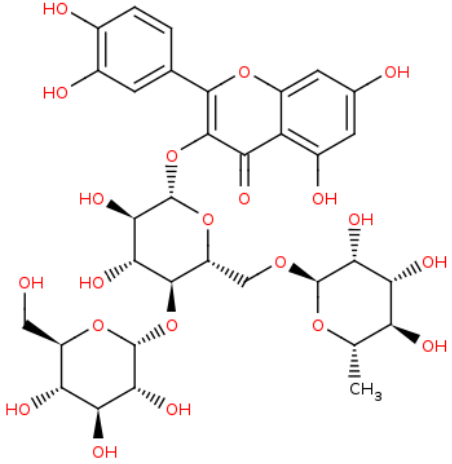
87-44-5			EC number 201-746-1
111879-80-2			EC number 422-320-3

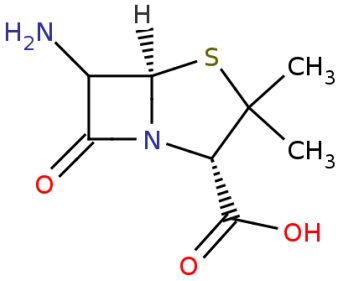
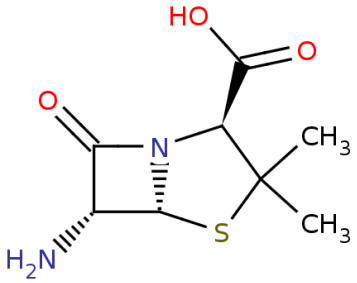
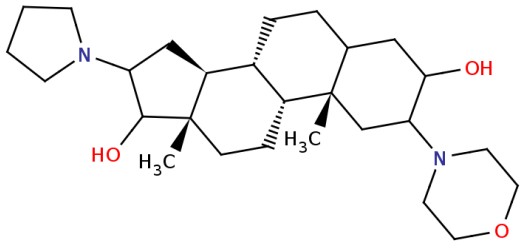
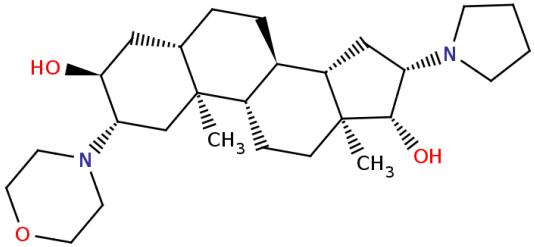
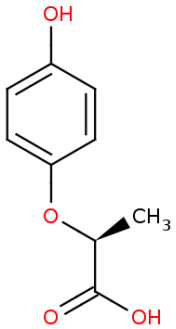
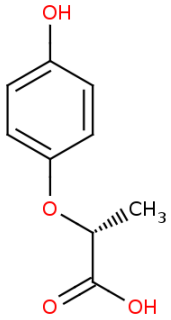
1380163-91-6 (incorrect form)		EC number 443-910-7
1380163-91-6 (correct form)		EC number 443-910-7

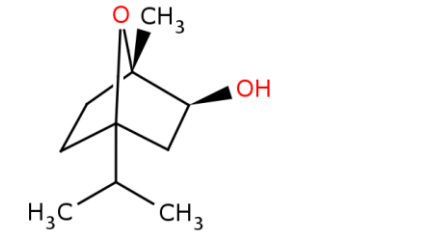
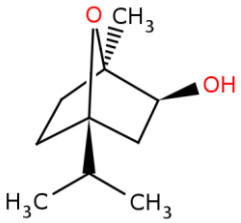
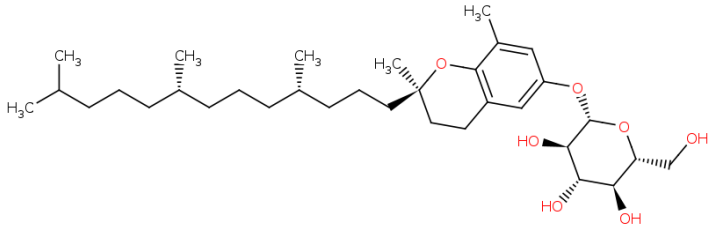
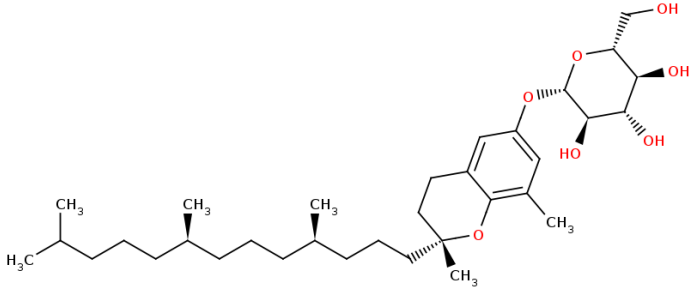
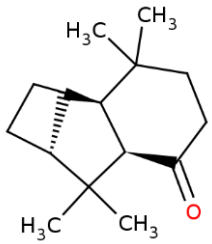
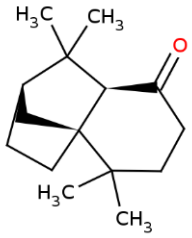
5) Inconsistencies related to the stereochemistry (deviating stereochemistry)

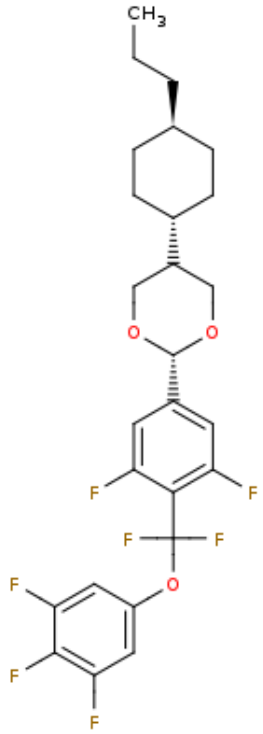
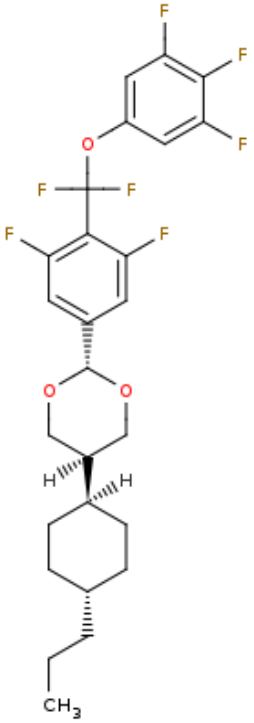
Table 5: Substances in the ECHA database where the SMILES do not correspond to the CAS RN™ as allocated in SciFindern. The reason for the mismatches here are deviations in the stereochemistry.

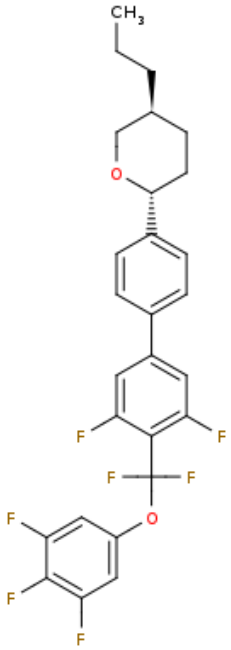
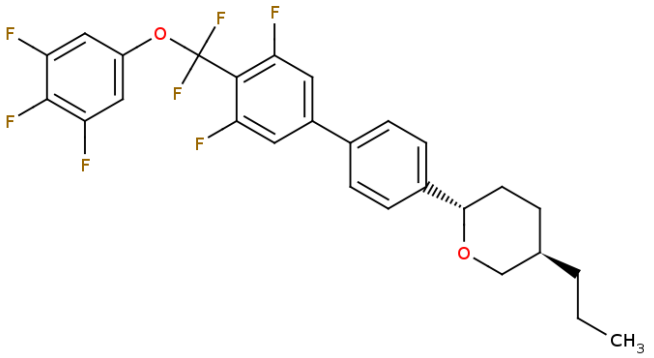
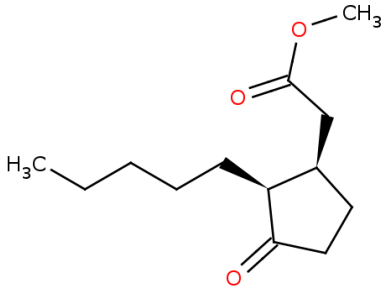
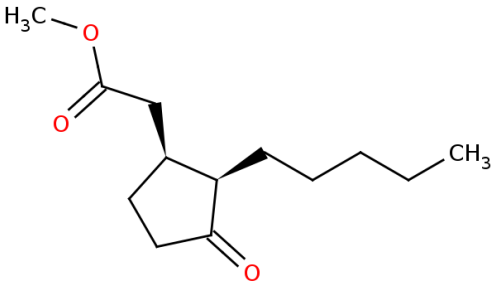
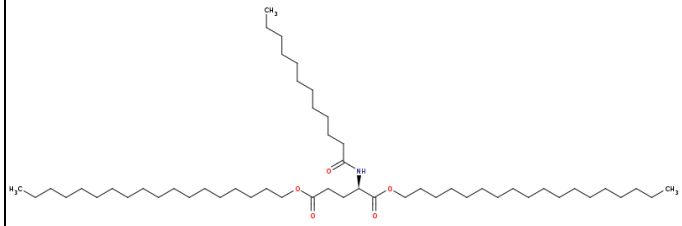
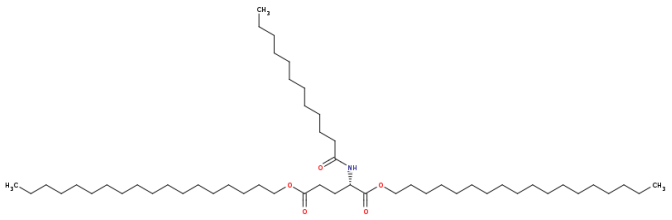
CAS RN™	Structure in the database	Structure corresponding to the CAS RN™	Comment
89-80-5			EC number 201-941-1
933-48-2			EC number 213-268-0
93183-15-4			EC number 685-519-6

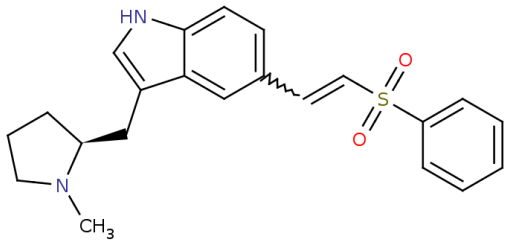
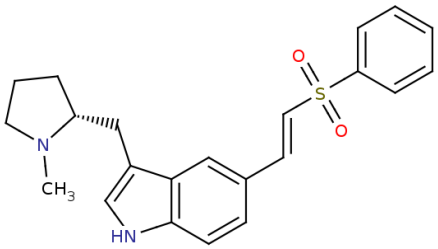
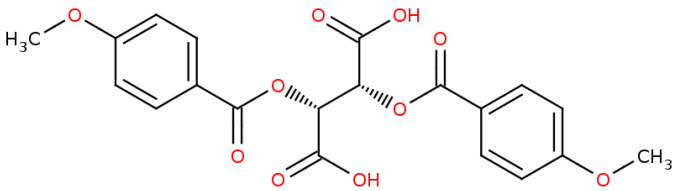
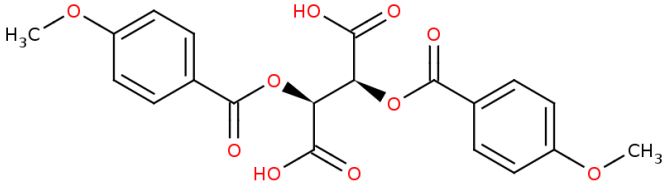
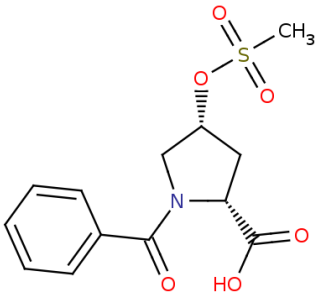
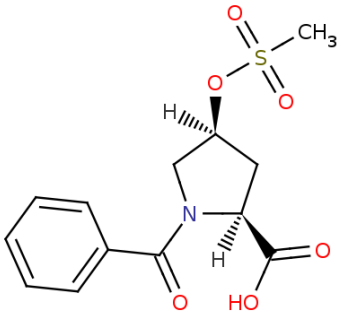
67219-55-0			EC number 266-605-9
130603-71-3			EC number 424-170-4

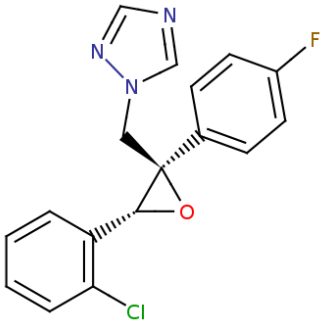
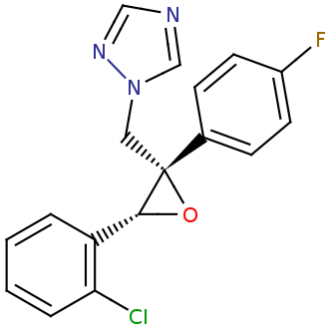
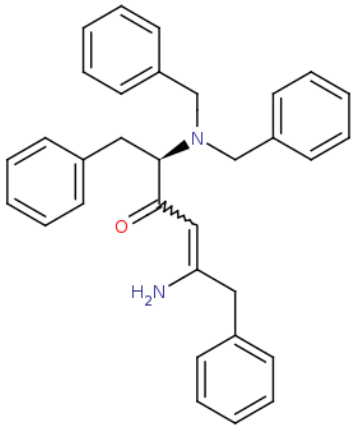
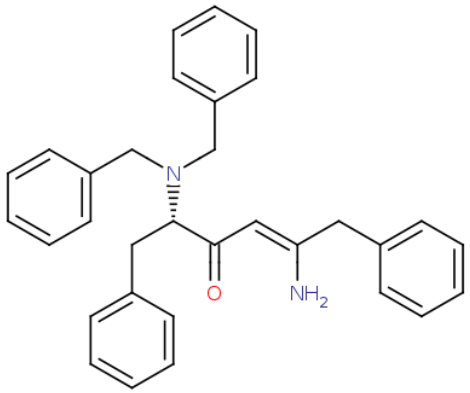
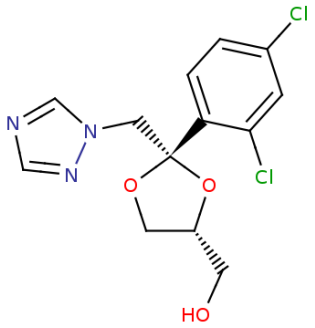
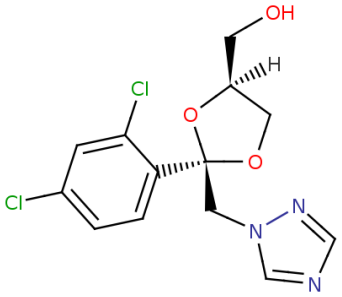
551-16-6			EC number 208-993-4
119302-20-4			EC number 601-595-5
94050-90-5			EC number 407-960-3

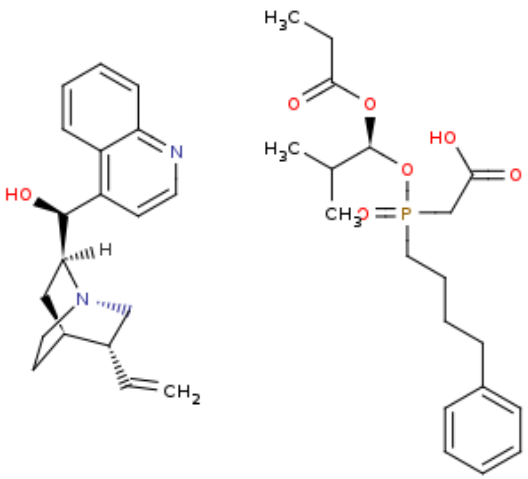
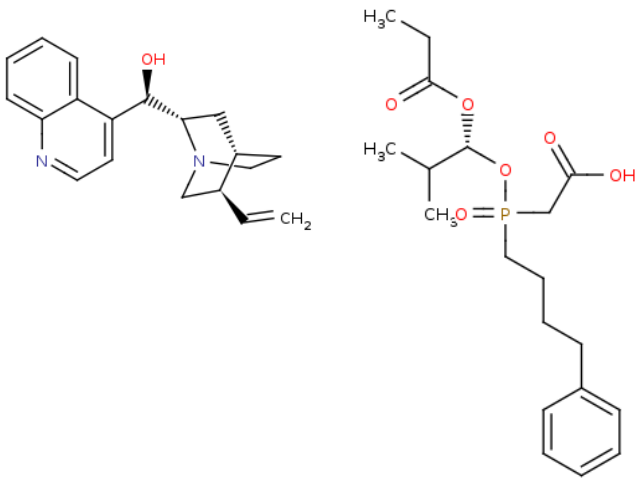
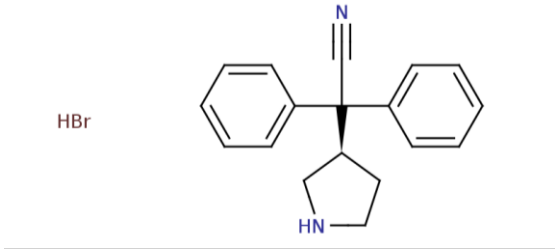
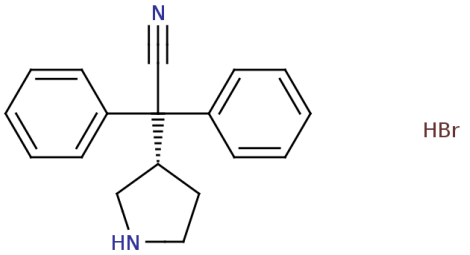
87172-89-2			EC number 402-470-6
102340-61-4			EC number 805-675-2
29461-13-0			EC number 249-648-8

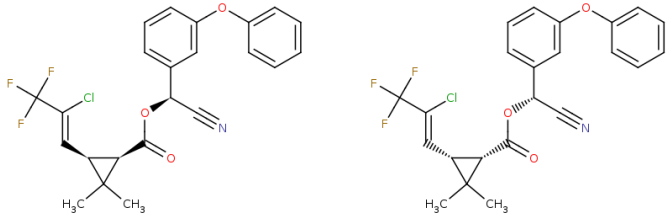
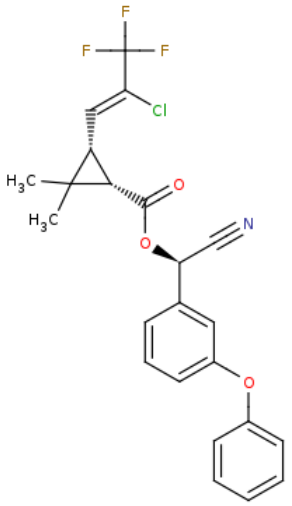
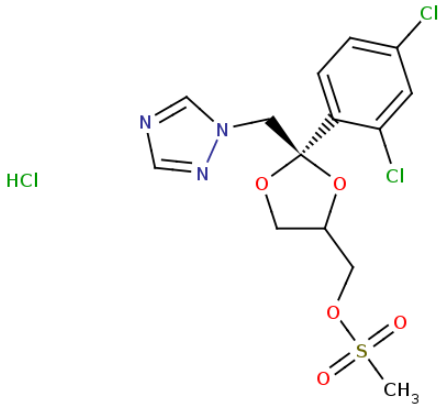
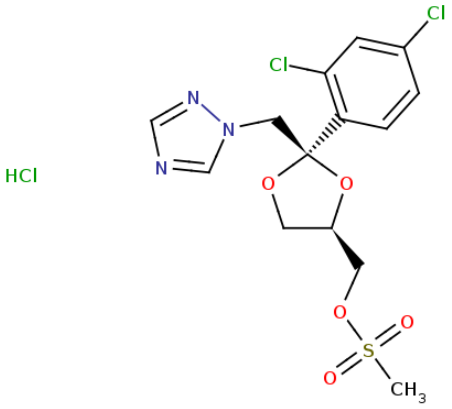
798556-07-7			EC number 700-701-8

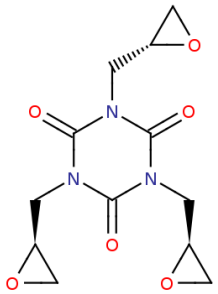
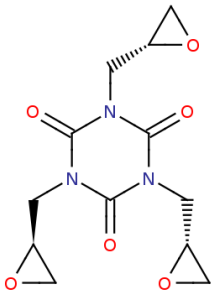
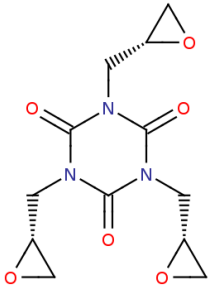
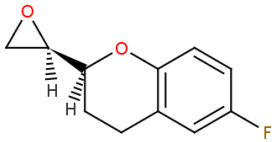
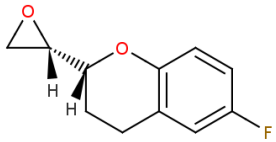
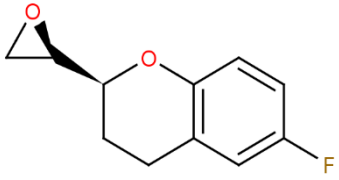
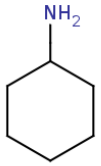
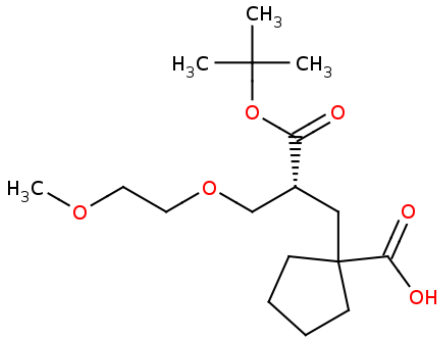
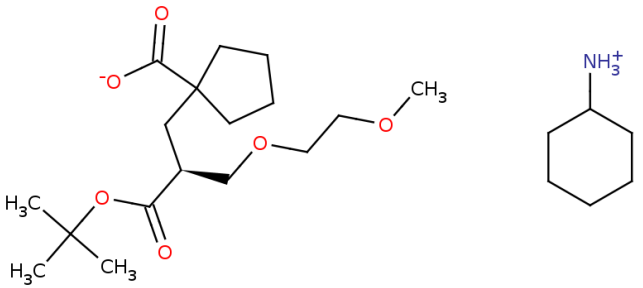
700863-48-5			EC number 615-063-5
93452-03-0			EC number 810-495-2
55258-21-4			EC number 807-033-7

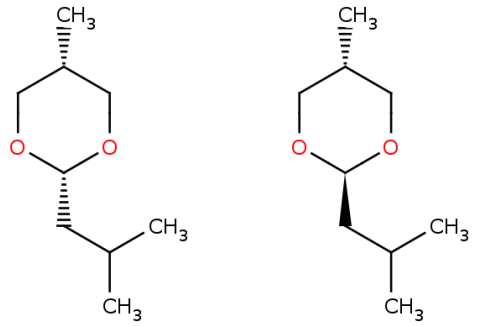
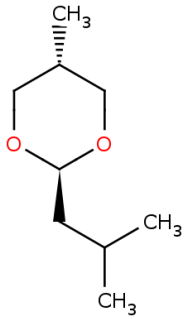
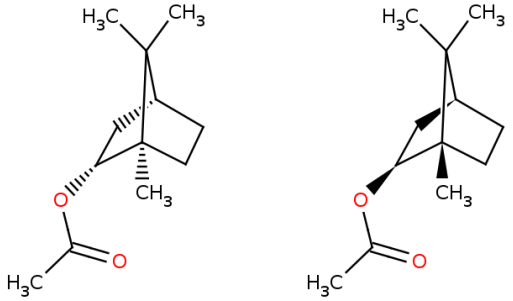
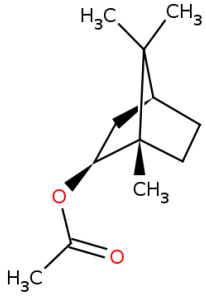
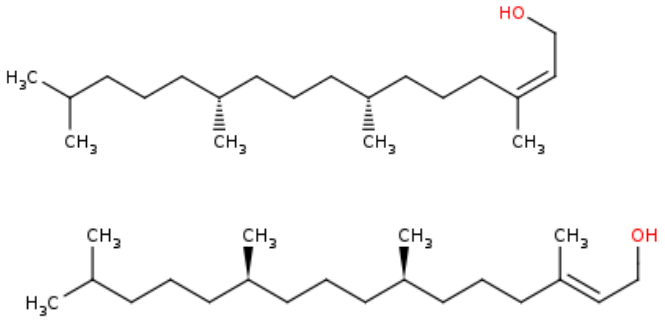
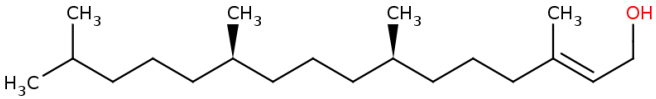
180637-89-2			EC number 430-560-5
191605-10-4			EC number 471-150-6
120807-02-5			EC number 416-040-0

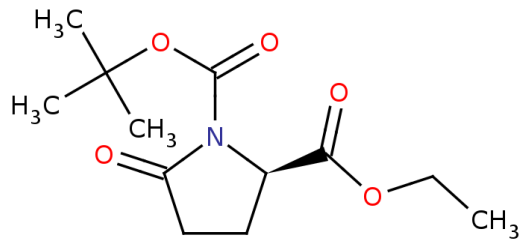
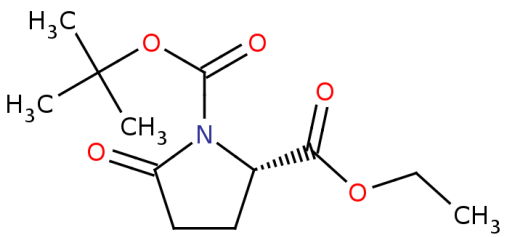
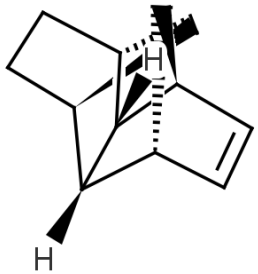
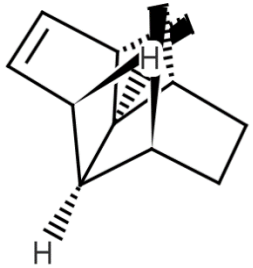
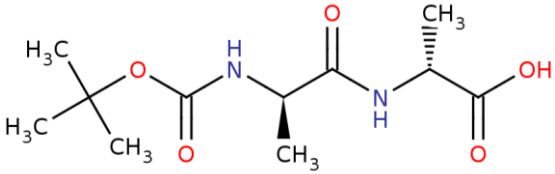
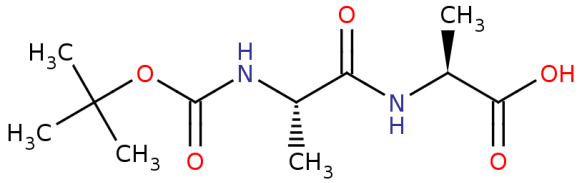
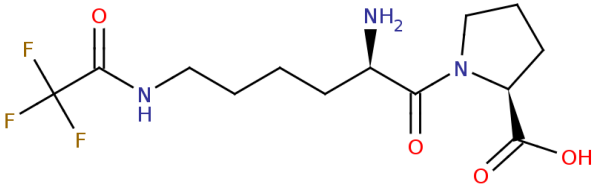
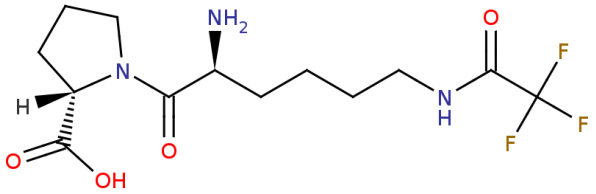
133855-98-8			EC number 406-850-2
156732-13-7			EC number 423-090-7
67914-85-6			EC number 267-747-4

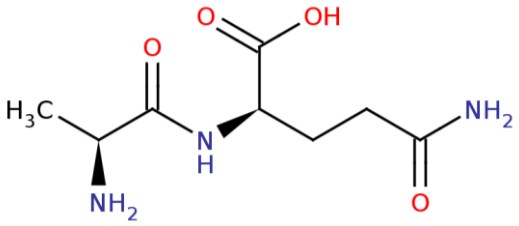
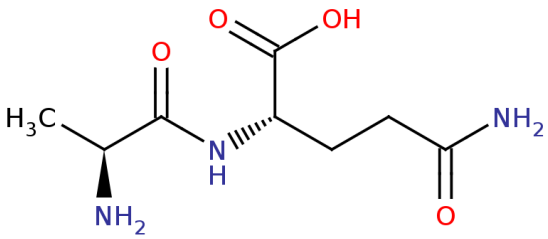
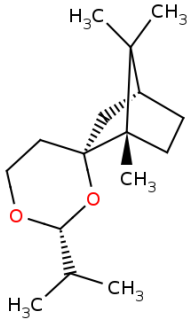
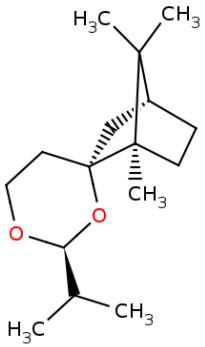
137590-32-0			EC number 415-820-8 both molecules differ
194602-27-2			EC number 421-810-4

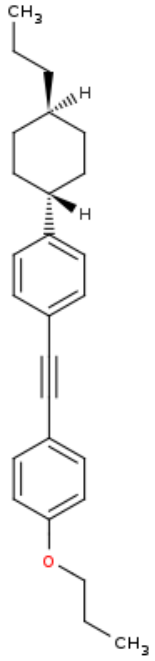
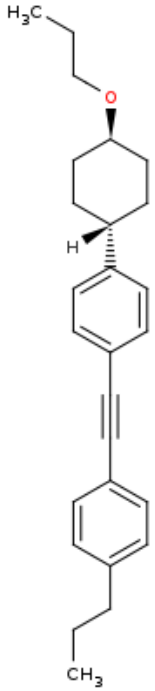
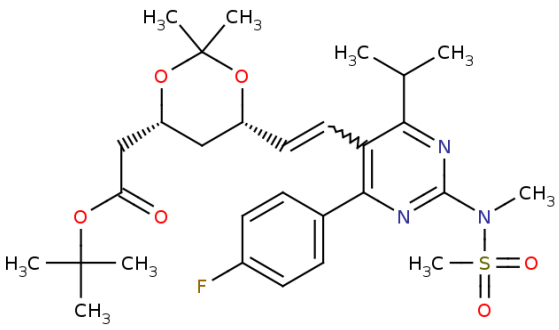
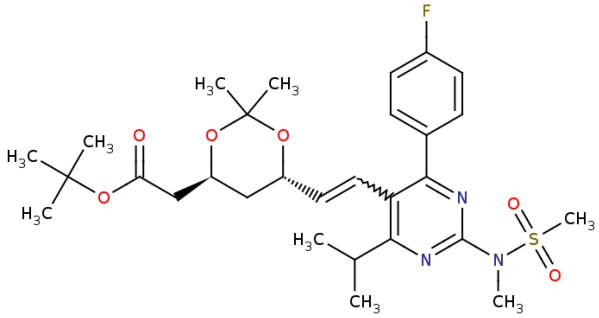
91465-08-6			EC number 415-130-7 the left molecule is different, the right molecule the same as the one in SciFinder[n]
155661-07-7			EC number 445-550-6

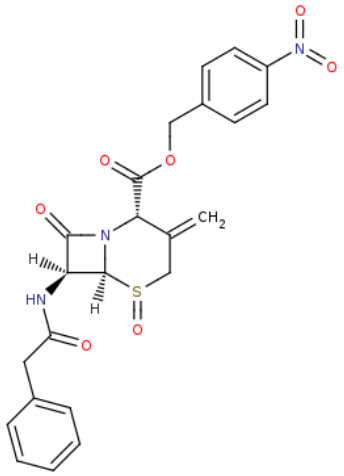
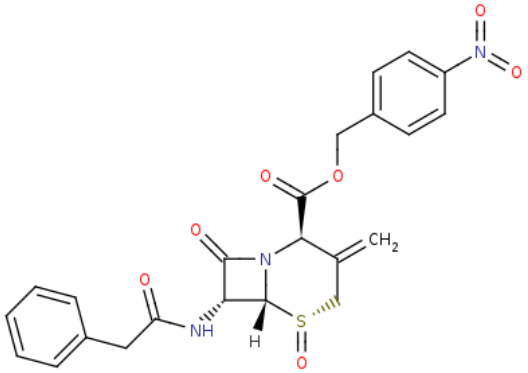
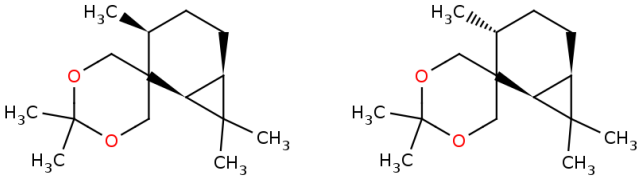
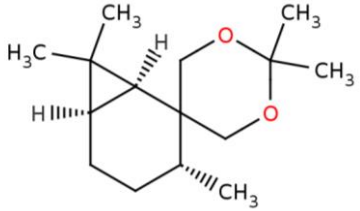
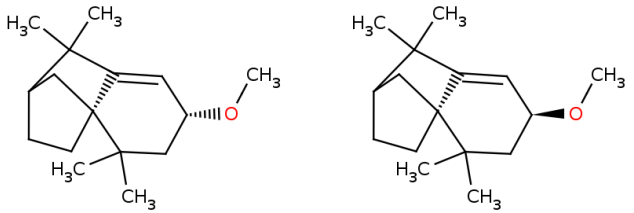
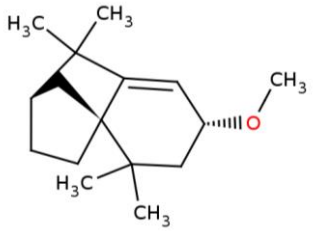
59653-74-6	 		EC number 423-400-0 both forms are in correct
793669-26-8	 		EC number 419-630-6 The CAS no. does not cover both forms. The left one is correct
167944-94-7	 		EC number 425-510-4

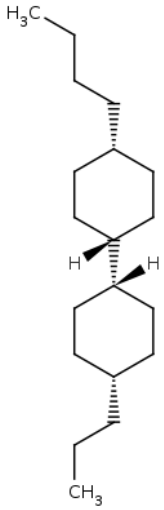
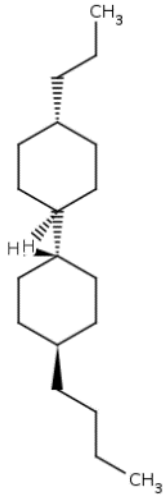
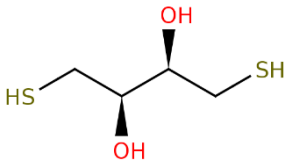
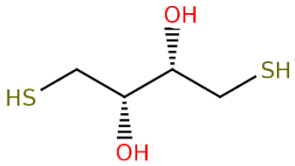
166301-21-9			EC number 426-130-1
125-12-2			EC number 204-727-6
150-86-7			EC number 416-120-5

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			EC number 475-290-9
188199-50-0			EC number 443-460-1

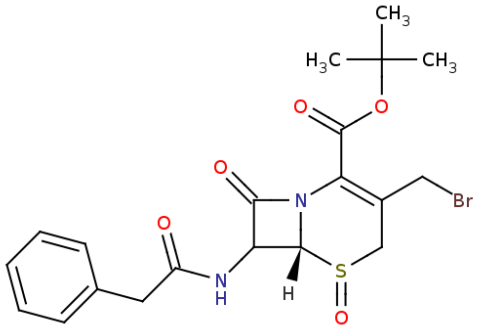
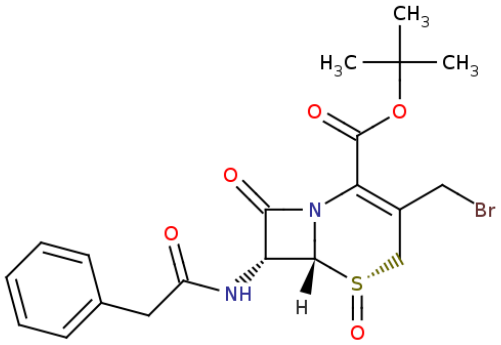
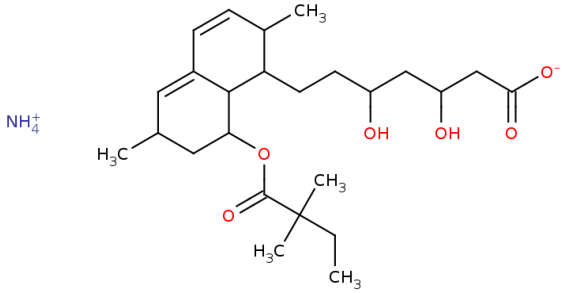
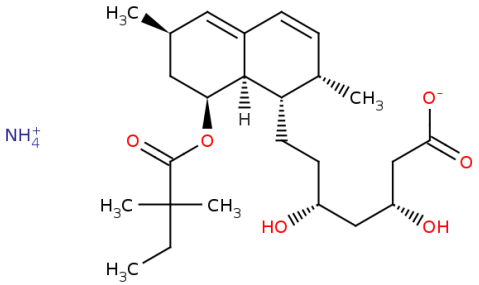
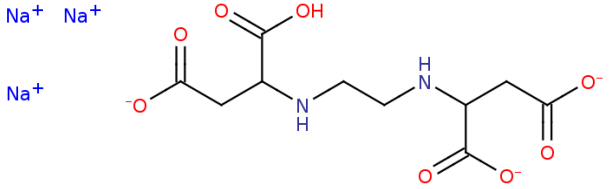
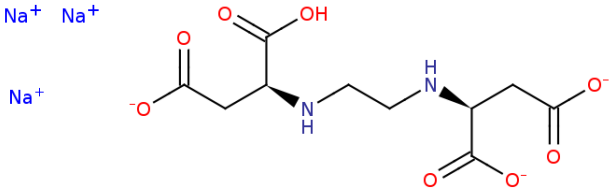
348113-98-4			EC number 448-430-1
1379976-09-6			EC number 432-810-9

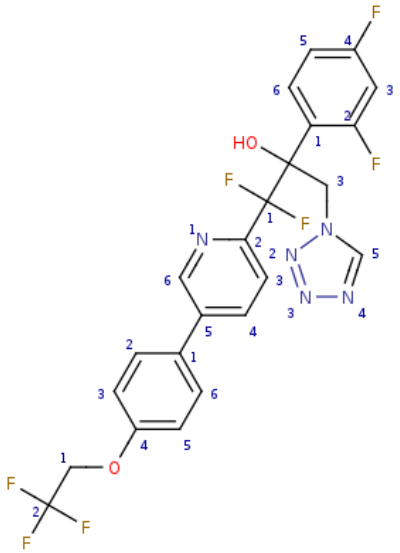
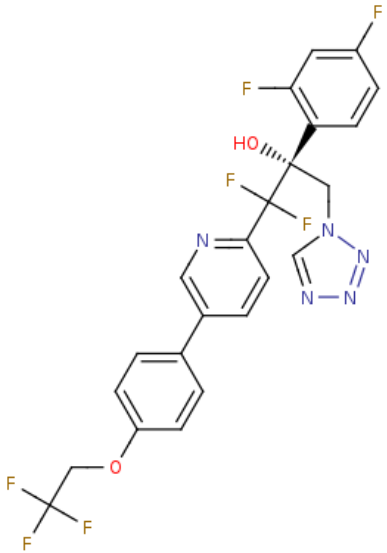
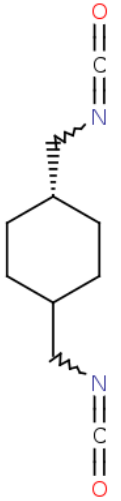
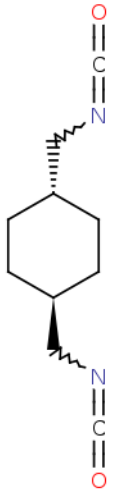
76109-32-5			EC number 412-800-0
121251-67-0			EC number 416-930-9
393517-29-8			EC number 444-480-3

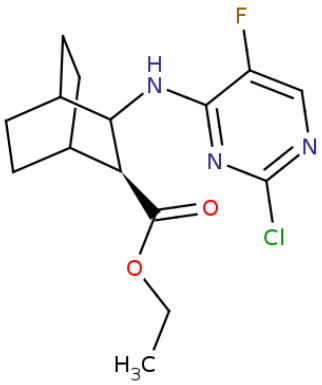
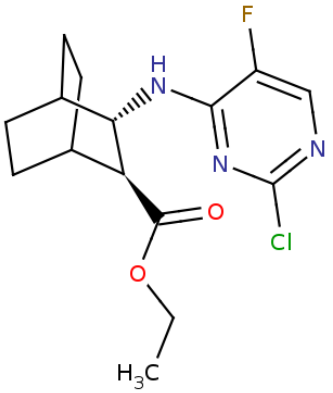
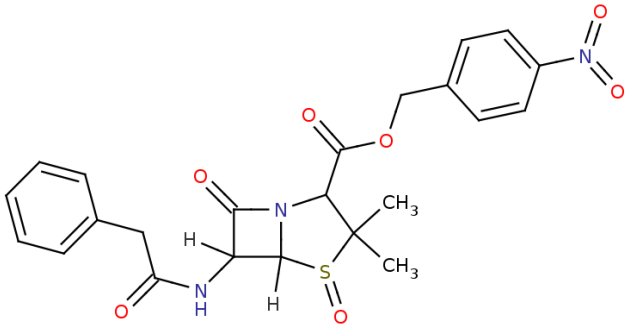
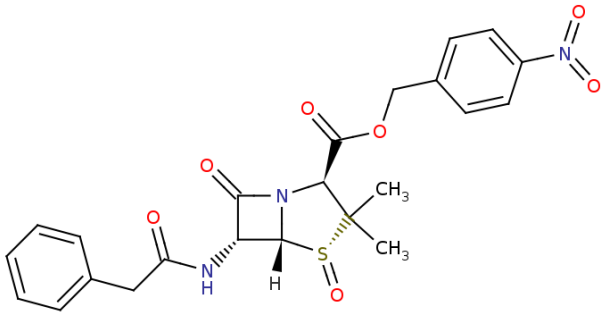
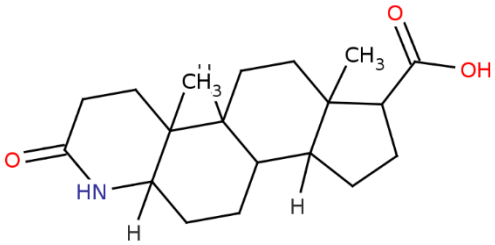
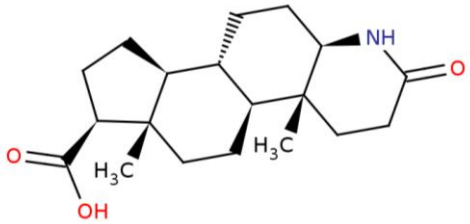
96624-52-1			EC number 619-232-4
3483-12-3			EC number 222-468-7

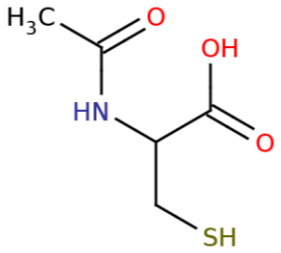
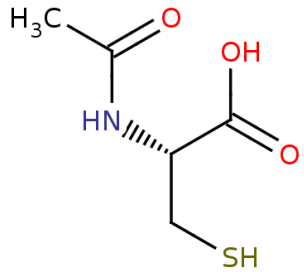
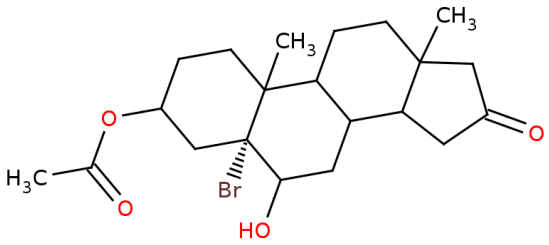
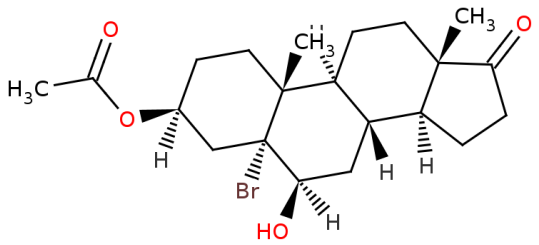
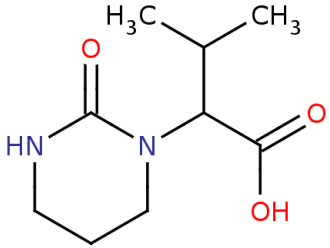
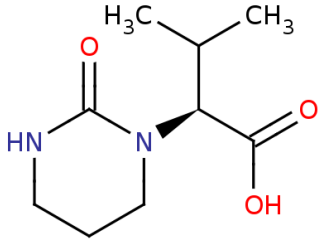
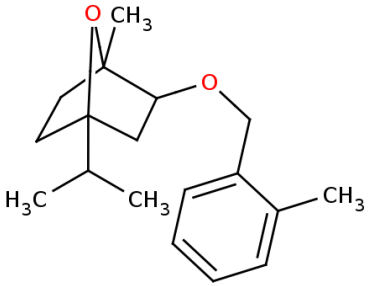
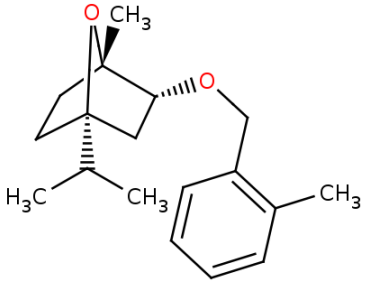
6) Inconsistencies related to the stereochemistry (no stereochemistry information in the ECHA database while SciFinder^n has some)

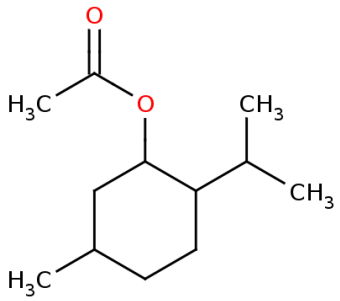
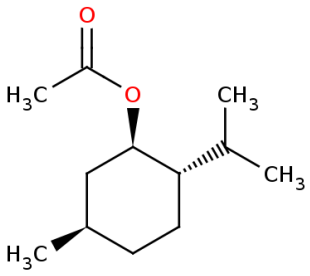
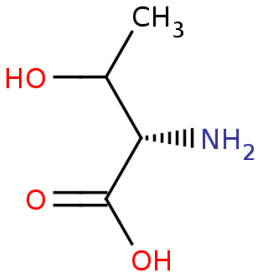
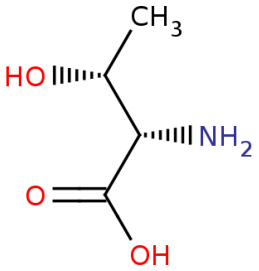
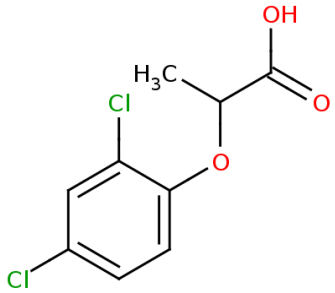
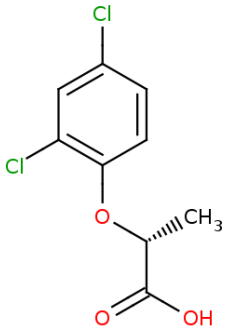
Table 6: Substances in the ECHA database where the SMILES do not correspond to the CAS RN™ as allocated in SciFindern. The reason for the mismatches here are stereochemistry information that are not available in the ECHA database while SciFindern has some.

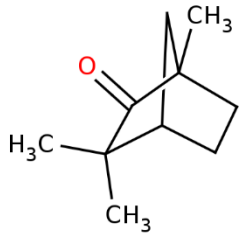
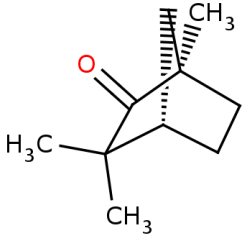
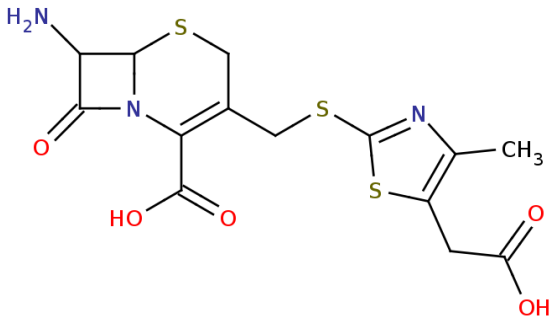
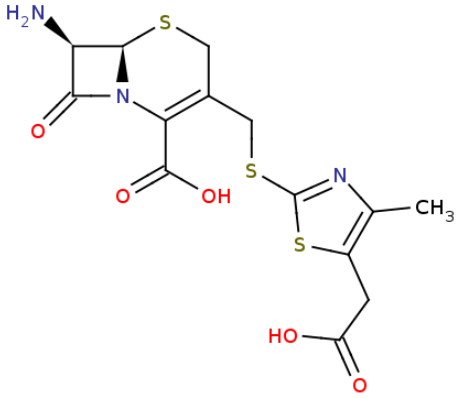
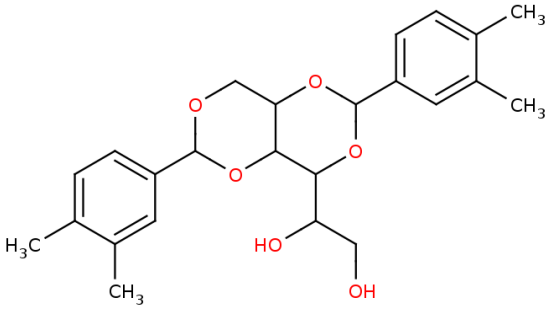
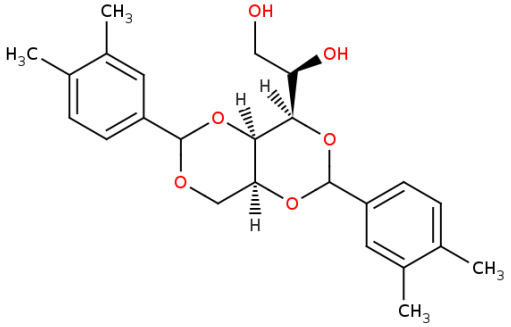
CAS RN™	Structure in the database	Structure corresponding to the CAS RN™	Comment
33610-13-8			EC number 407-620-4
139893-43-9			EC number 404-520-2
178949-82-1			EC number 416-530-4

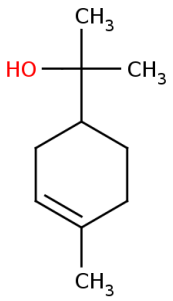
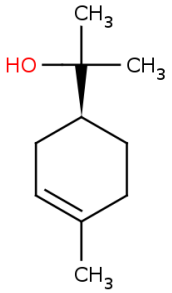
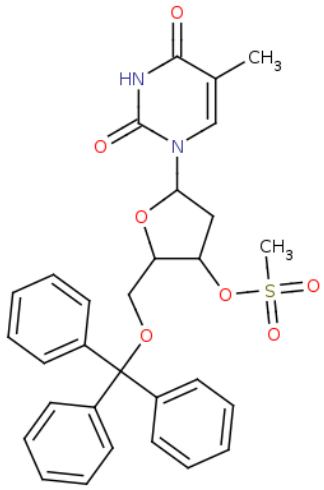
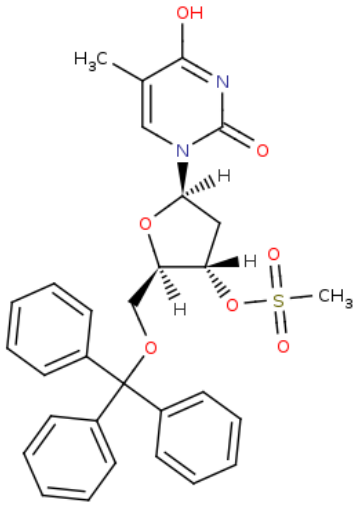
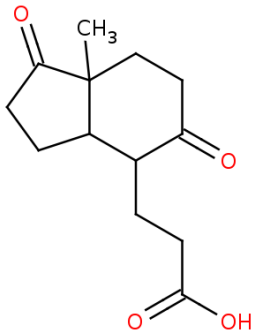
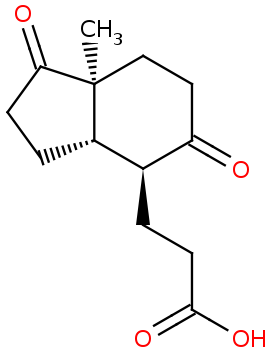
1340593-59-0			EC number 841-499-2
98458-83-4			EC number 825-609-6

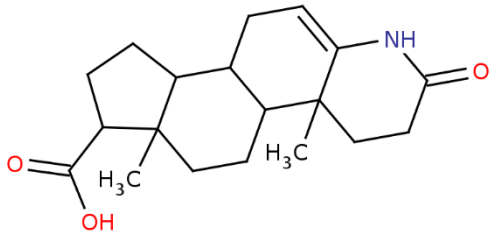
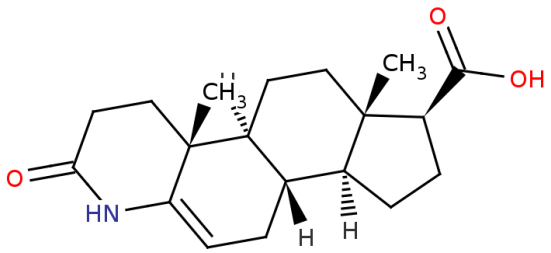
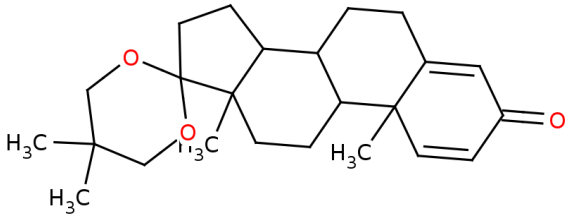
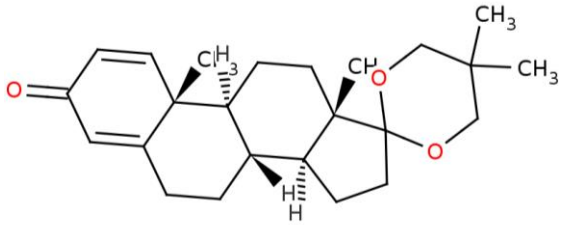
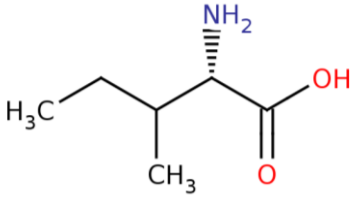
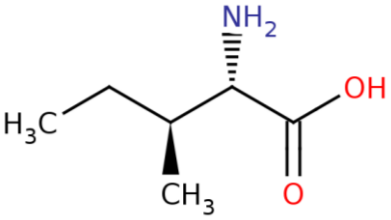
1777721-57-9			EC number 821-183-0
54275-93-3			EC number 412-670-5
103335-55-3			EC number 407-820-1

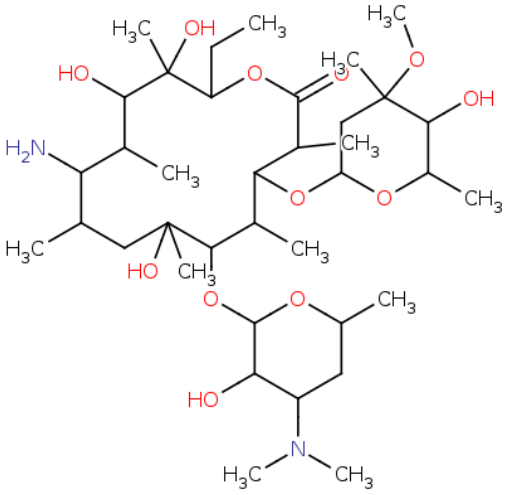
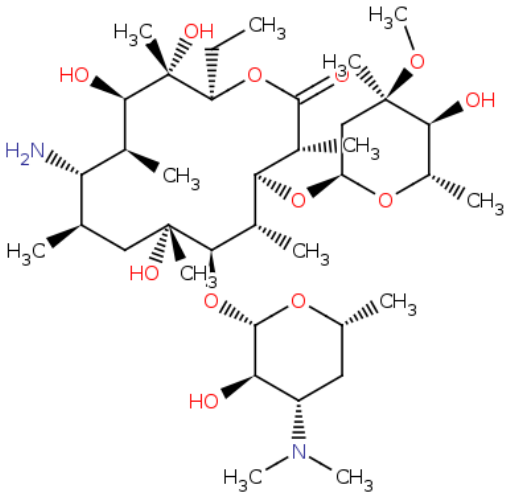
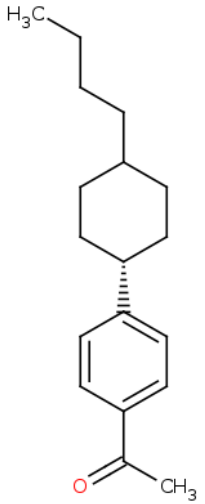
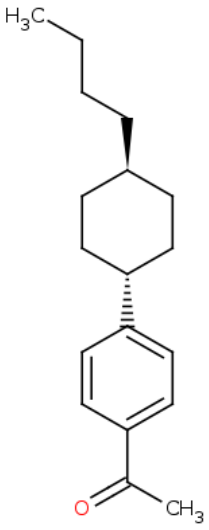
616-91-1			EC number 210-498-3
4229-69-0			EC number 419-790-7
192725-50-1			EC number 430-900-2
87818-31-3			EC number 402-410-9

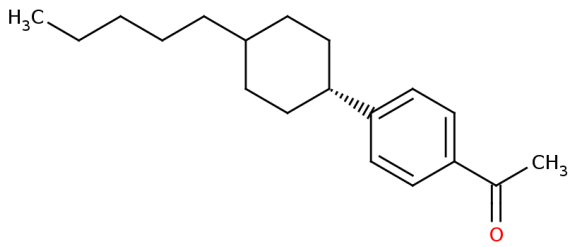
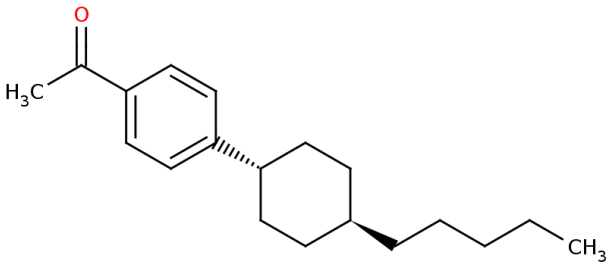
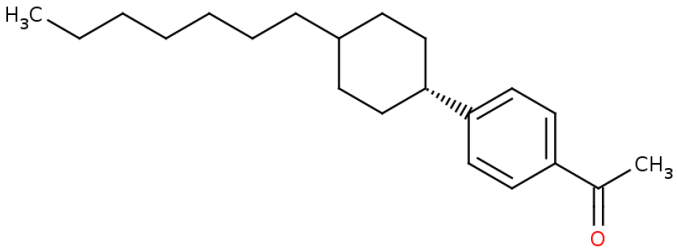
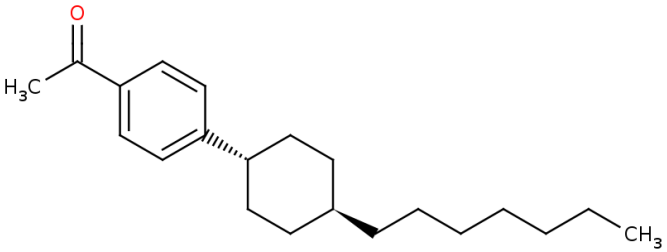
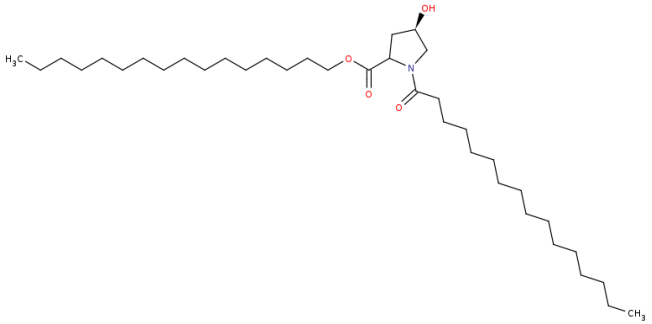
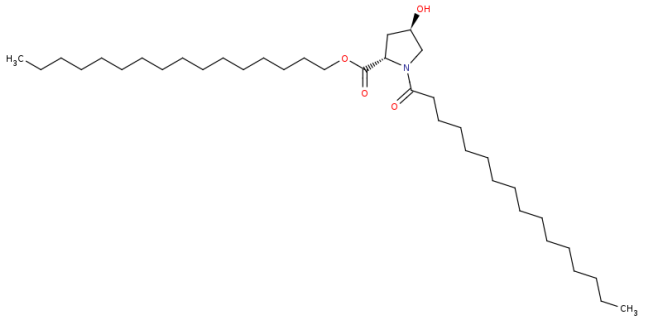
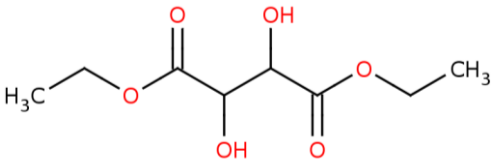
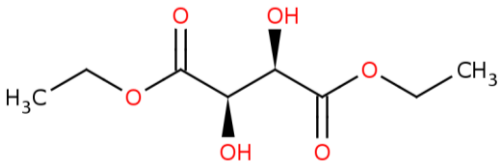
89-48-5			EC number 201-911-8
72-19-5			EC number 200-774-1
15165-67-0			EC number 403-980-1

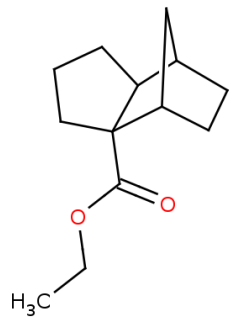
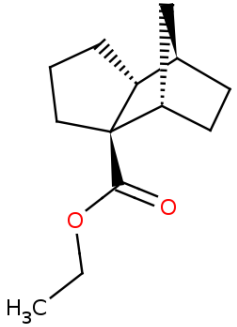
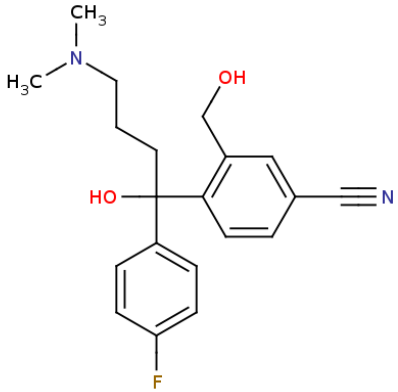
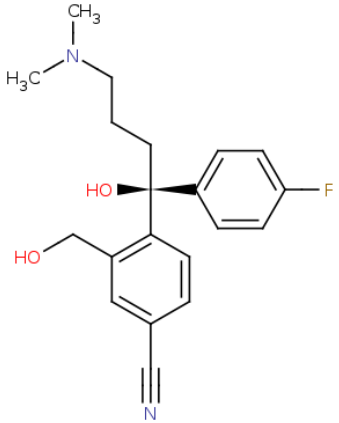
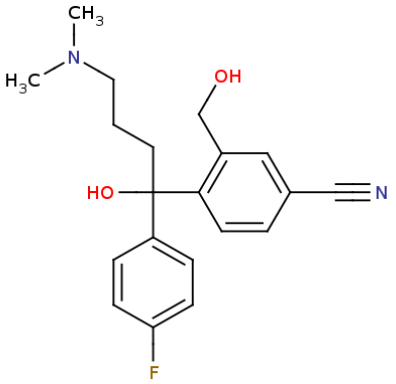
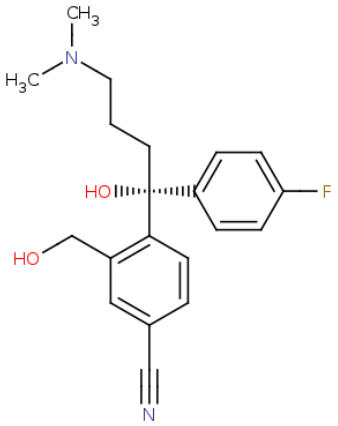
7787-20-4			EC number 232-107-5
111298-82-9			EC number 403-690-5
135861-56-2			EC number 413-110-2

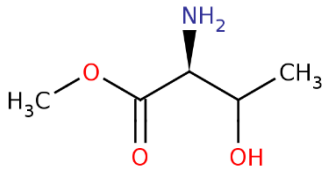
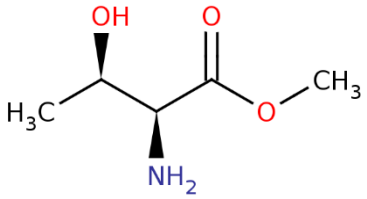
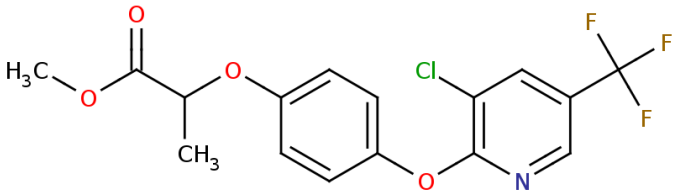
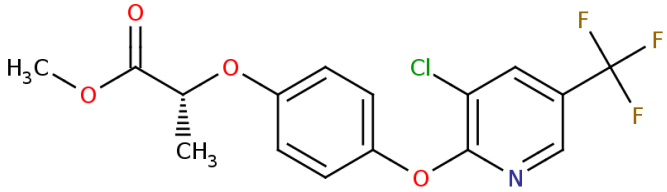
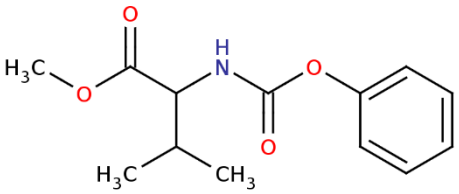
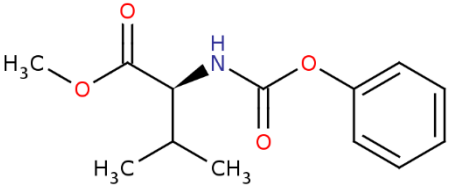
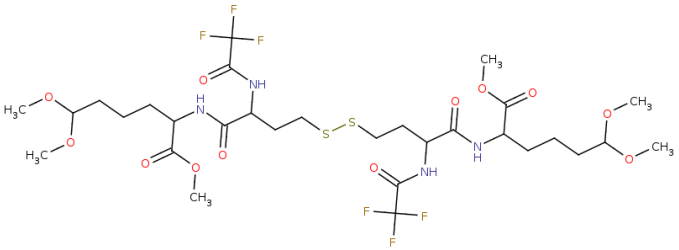
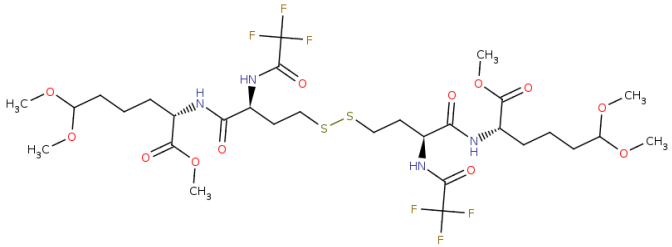
10482-56-1			EC number 233-986-8
104218-44-2			EC number 406-360-9
1944-63-4			EC number 435-830-6

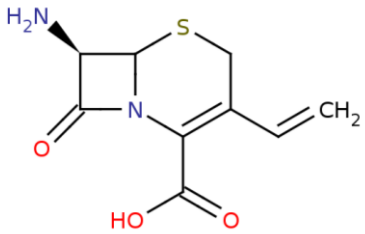
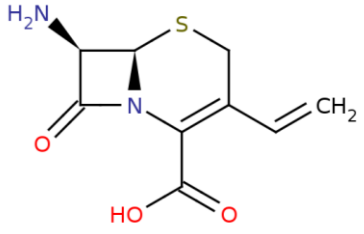
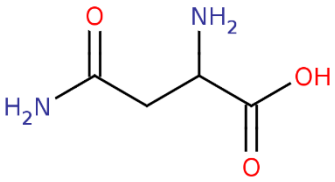
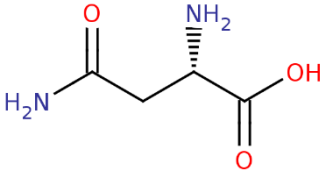
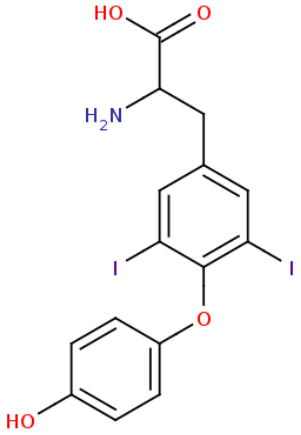
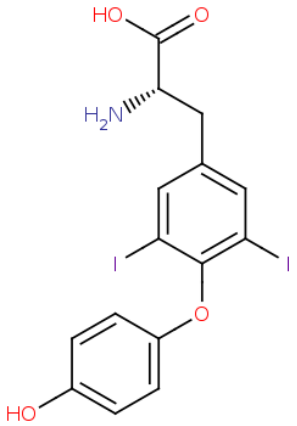
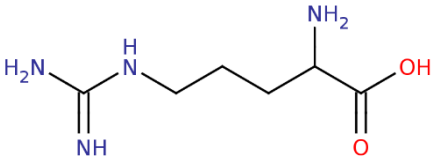
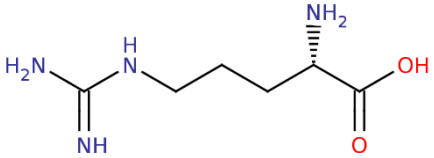
103335-54-2			EC number 407-830-6
13258-43-0			EC number 421-050-3
73-32-5			EC number 200-798-2

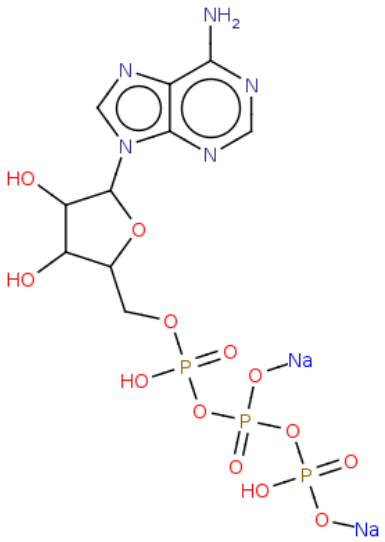
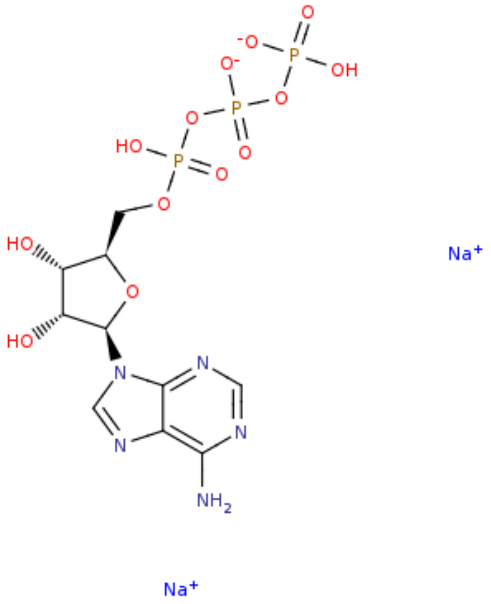
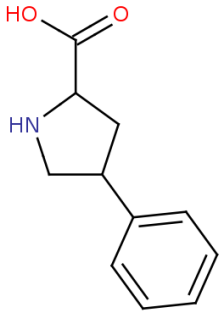
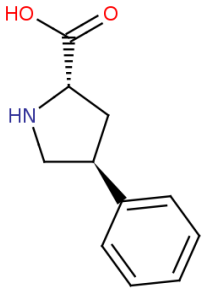
26116-56-3			EC number 406-790-7
83626-30-6			EC number 427-320-7

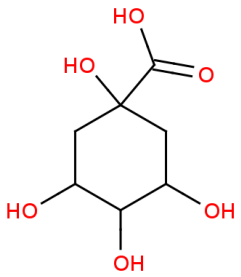
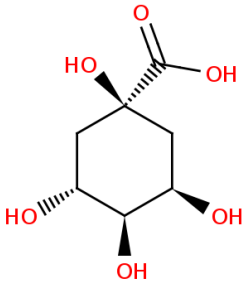
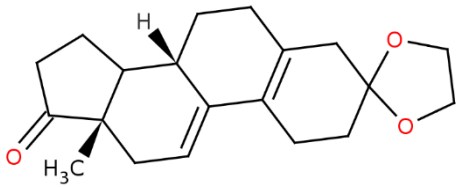
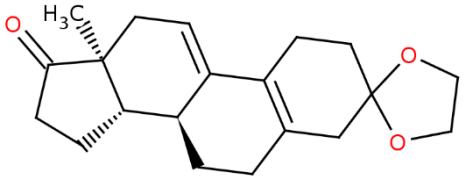
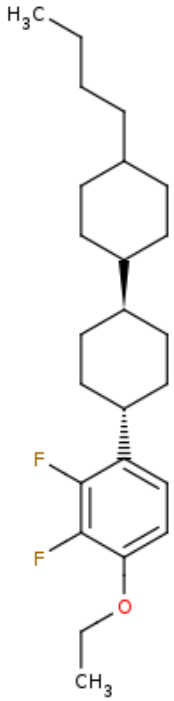
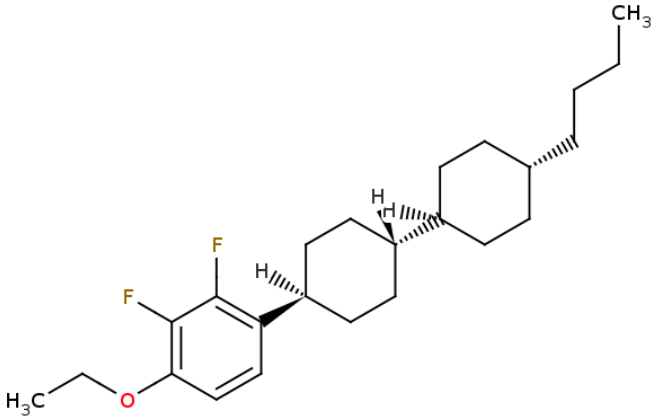
78531-59-6			EC number 426-830-7
78531-60-9			EC number 426-820-2
791838-11-4			EC number 479-990-5
87-91-2			EC number 201-783-3

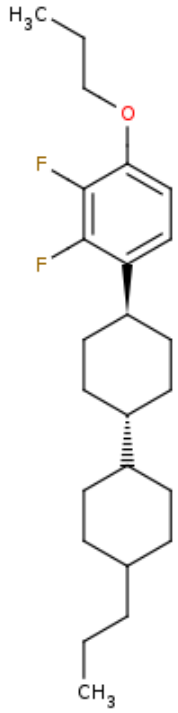
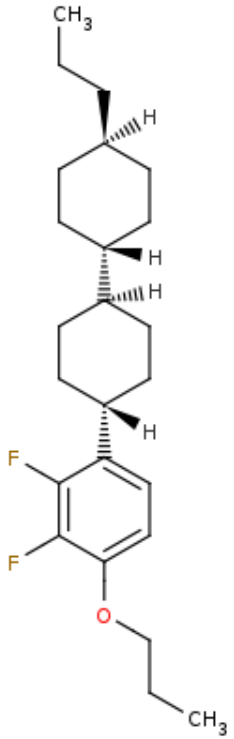
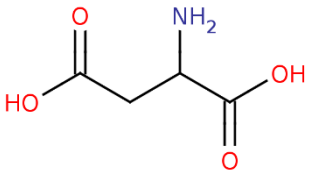
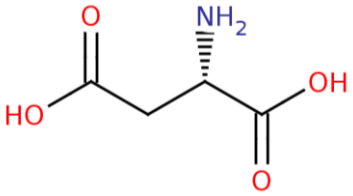
80657-64-3			EC number 407-520-0
128173-52-4			EC number 430-770-7
219861-18-4			EC number 430-760-2

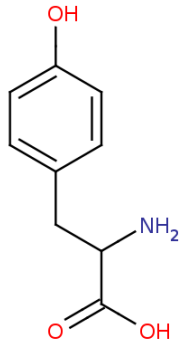
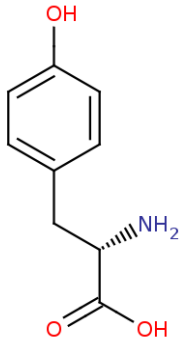
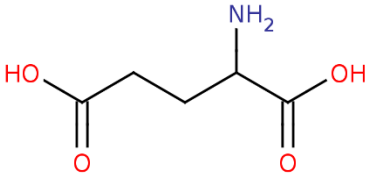
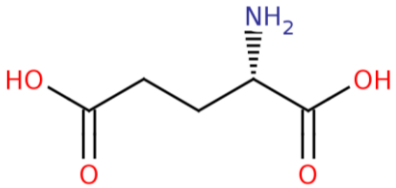
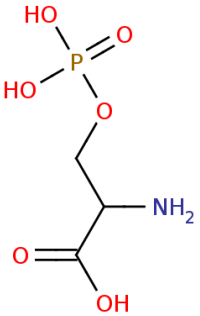
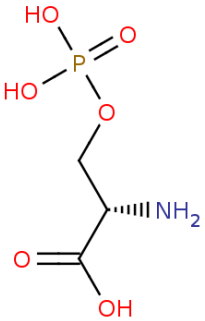
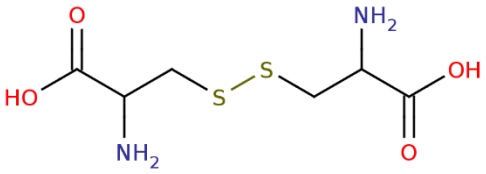
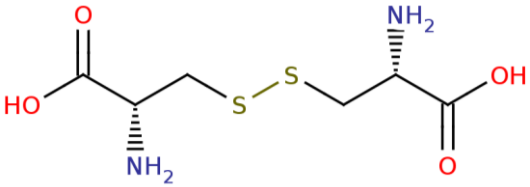
3373-59-9			EC number 222-158-1
72619-32-0			EC number 406-250-0
153441-77-1			EC number 414-500-5
255387-46-3			EC number 432-860-1

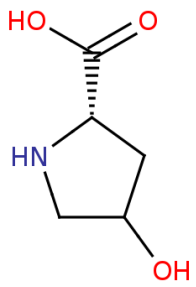
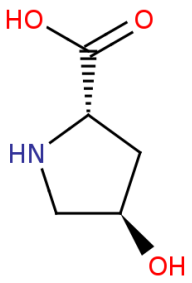
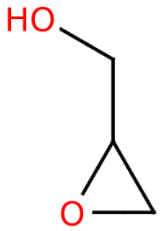
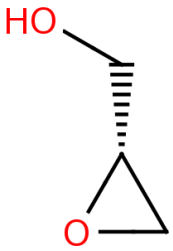
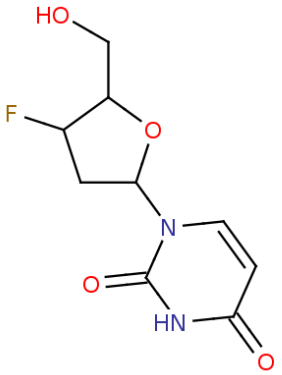
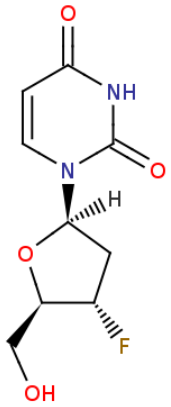
79349-82-9			EC number 438-350-5
70-47-3			EC number 200-735-9
1041-01-6			EC number 213-867-7
74-79-3			EC number 200-811-1

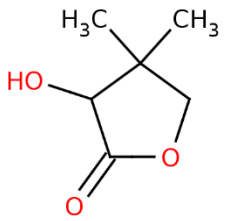
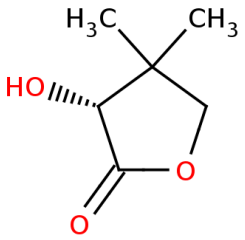
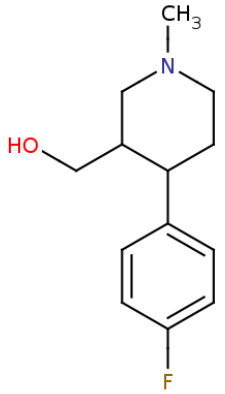
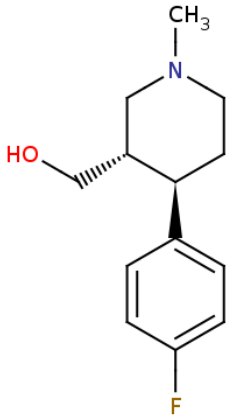
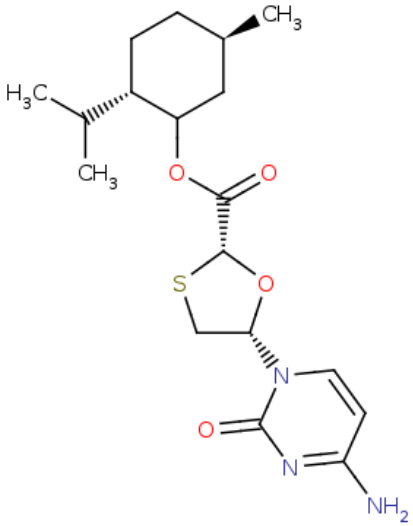
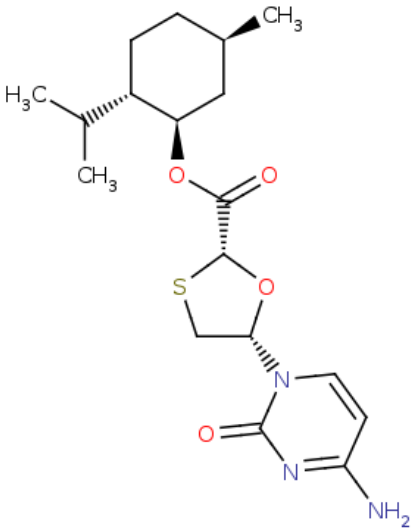
987-65-5			EC number 213-579-1
96314-26-0			EC number 416-020-1

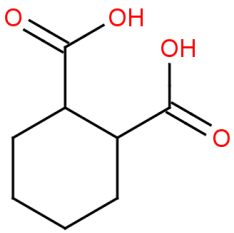
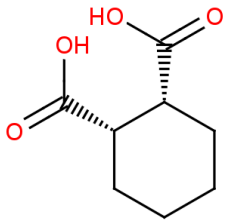
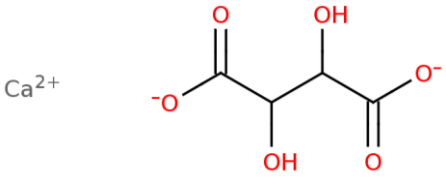
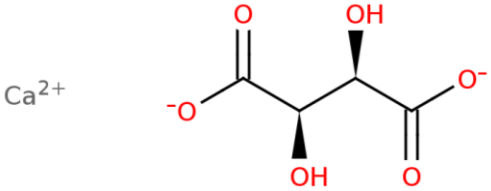
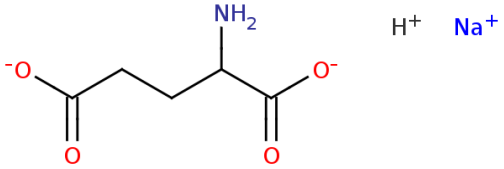
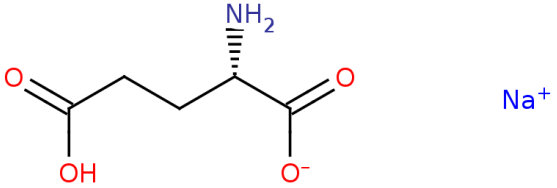
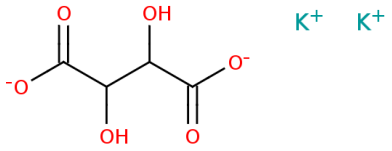
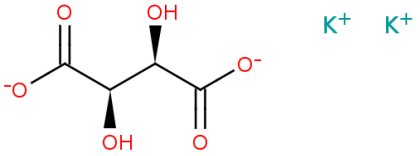
77-95-2			EC number 201-072-8
5571-36-8			EC number 427-230-8
473257-15-7			EC number 610-337-0

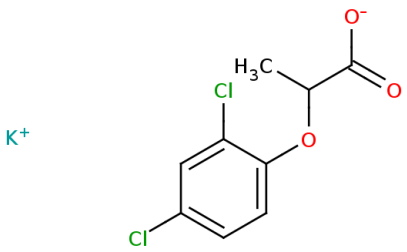
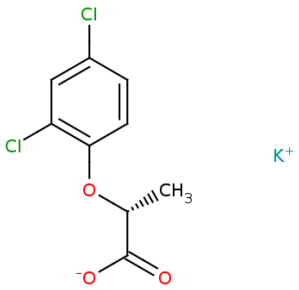
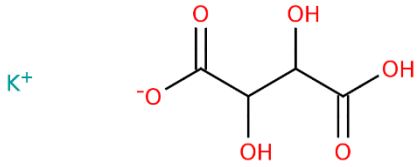
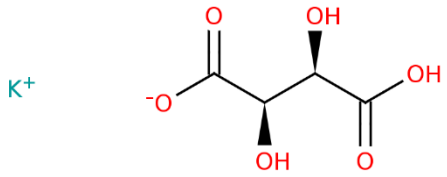
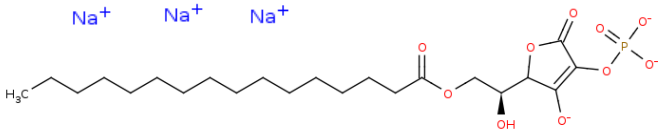
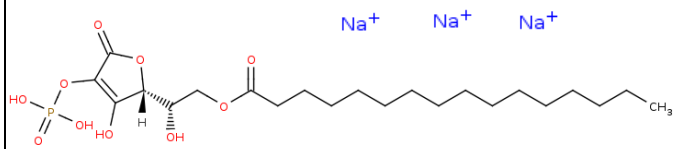
473257-14-6			EC number 610-336-5
56-84-8			EC number 200-291-6

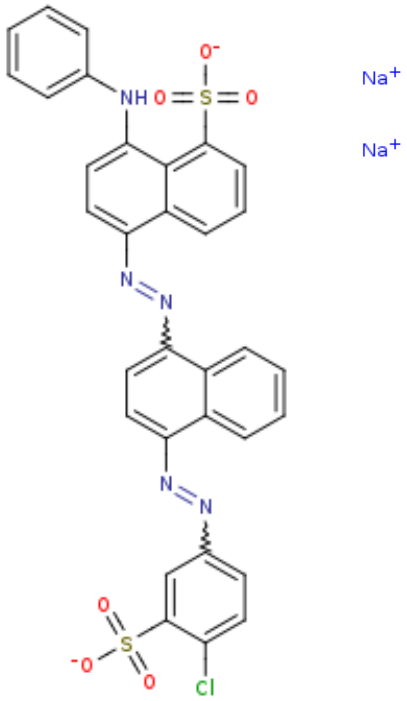
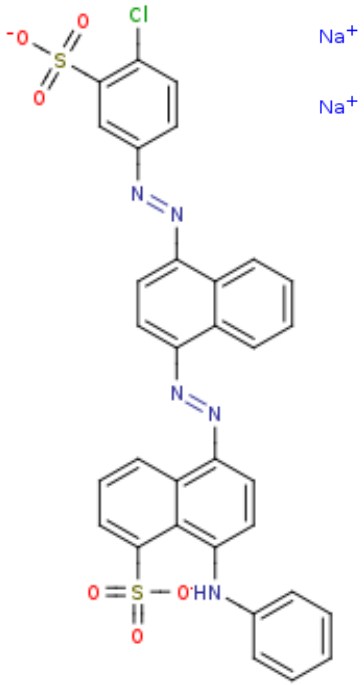
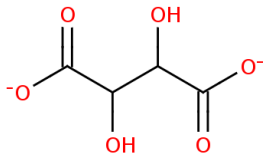
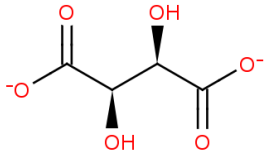
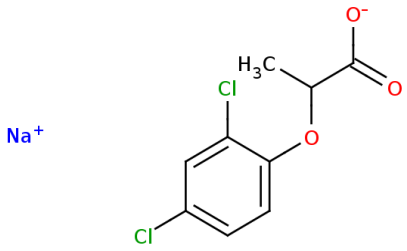
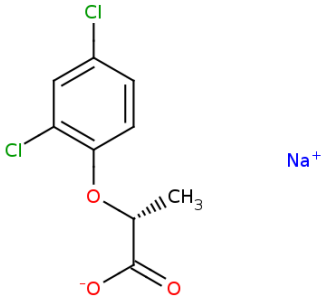
60-18-4			EC number 200-460-4
56-86-0			EC number 200-293-7
407-41-0			EC number 206-986-0
56-89-3			EC number 200-296-3

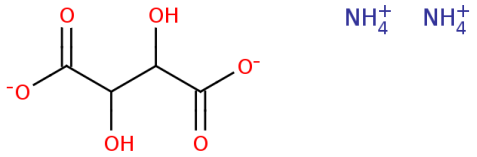
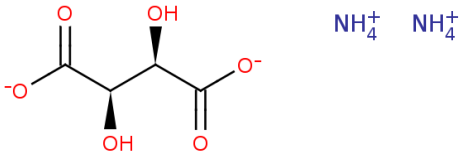
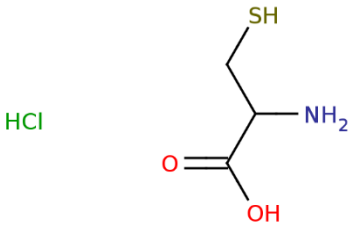
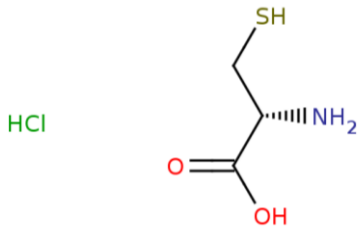
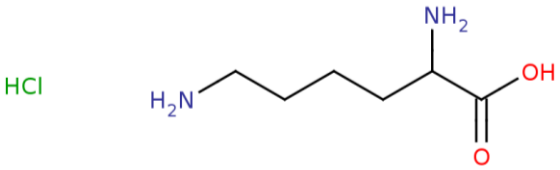
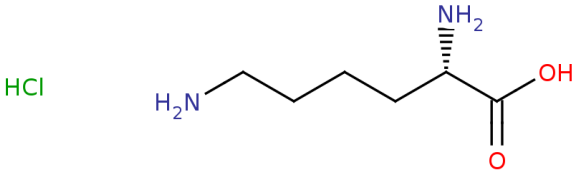
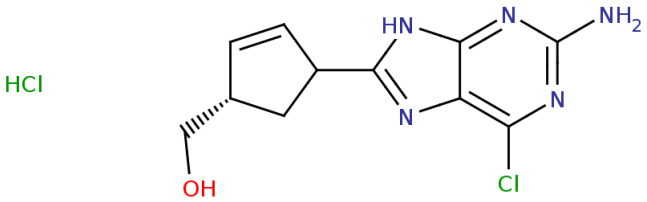
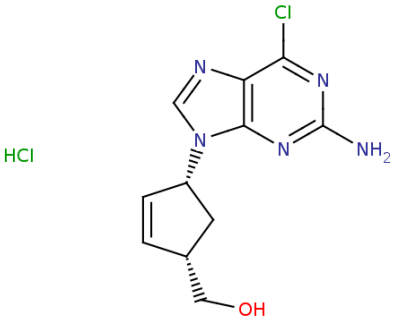
51-35-4			EC number 200-091-9
57044-25-4			EC number 404-660-4
41107-56-6			EC number 415-360-8

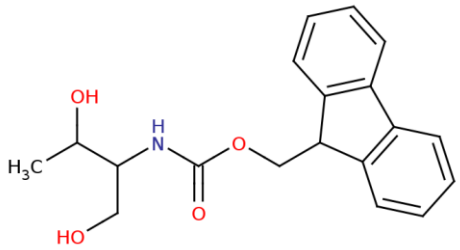
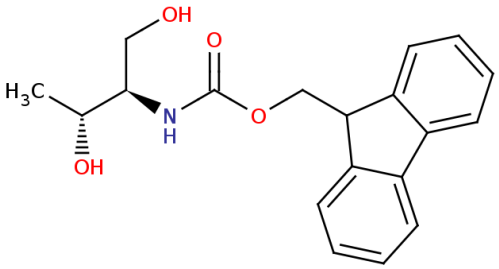
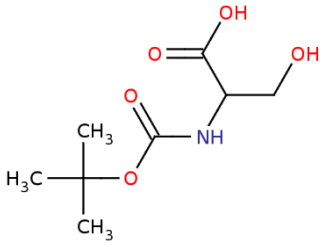
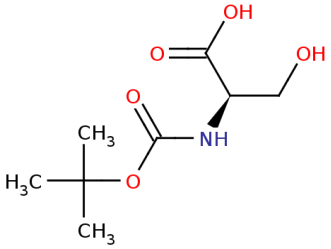
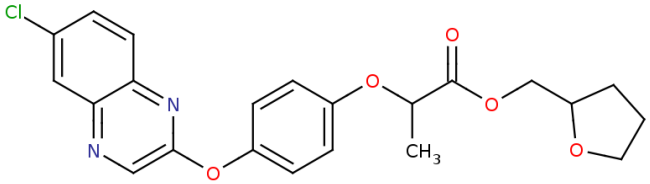
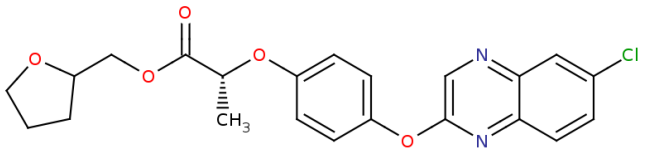
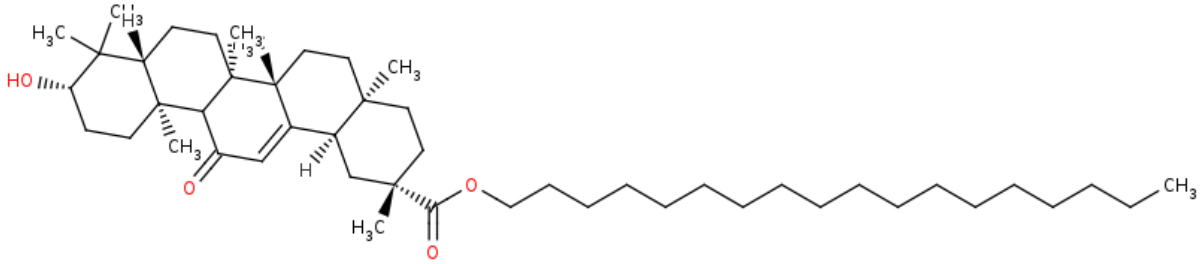
599-04-2			EC number 209-963-3
105812-81-5			EC number 406-030-4
147027-10-9			EC number 425-250-1

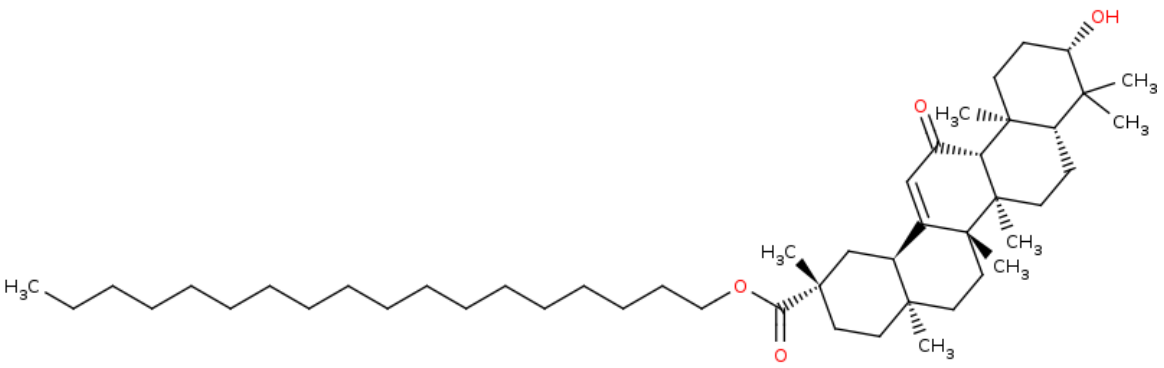
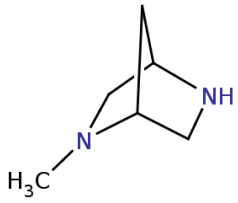
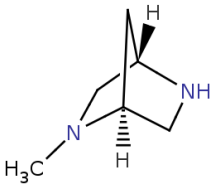
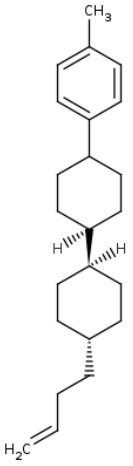
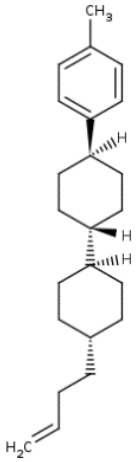
610-09-3			EC number 445-870-6
3164-34-9			EC number 221-621-5
142-47-2			EC number 205-538-1
921-53-9			EC number 213-067-8

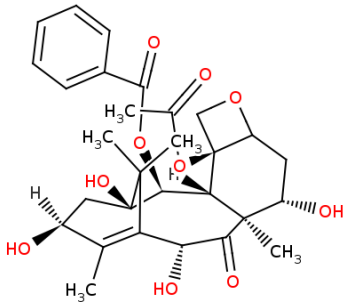
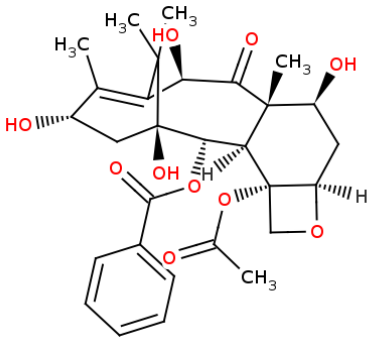
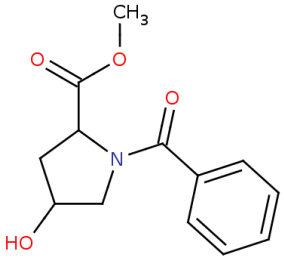
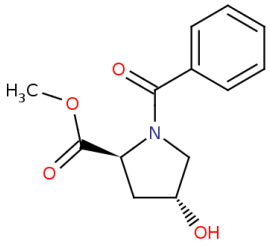
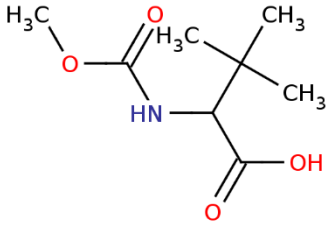
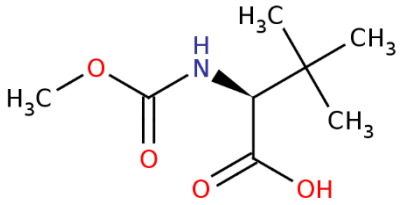
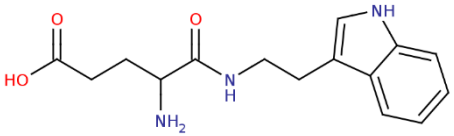
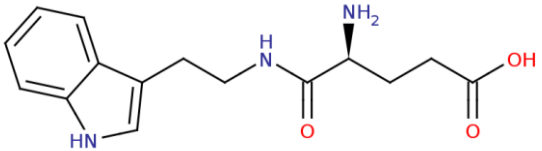
113963-87-4			EC number 413-580-9
868-14-4			EC number 212-769-1
302345-18-2			EC number 471-090-0

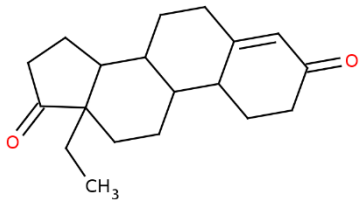
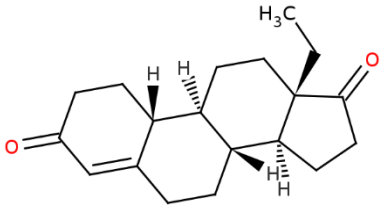
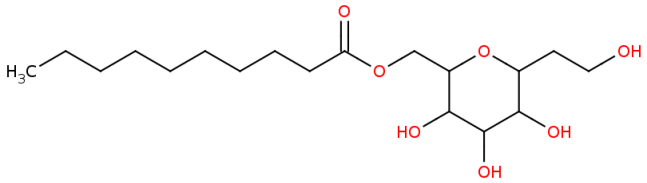
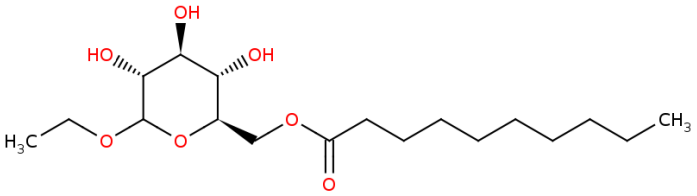
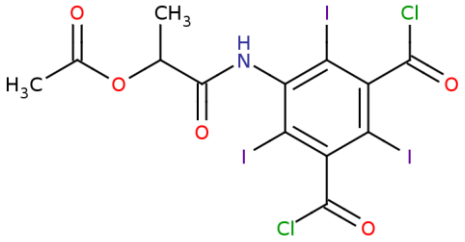
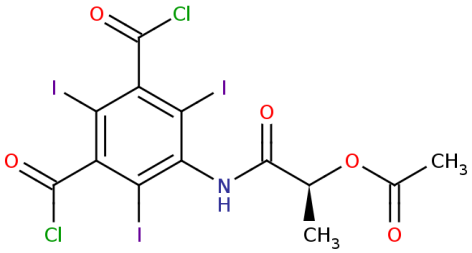
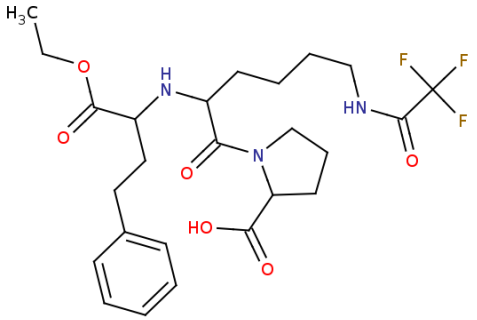
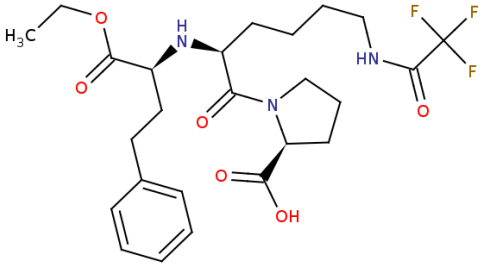
6527-62-4			EC number 413-600-6
868-18-8			EC number 212-773-3
119299-10-4			EC number 413-340-3

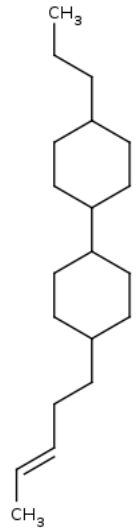
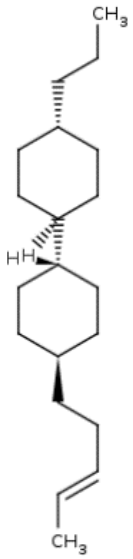
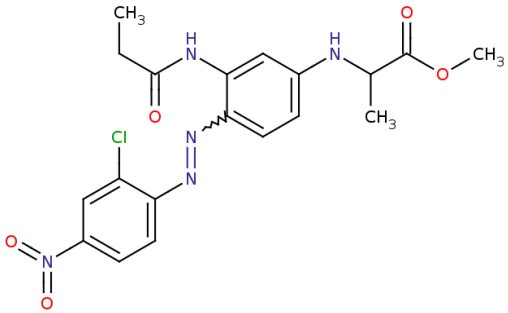
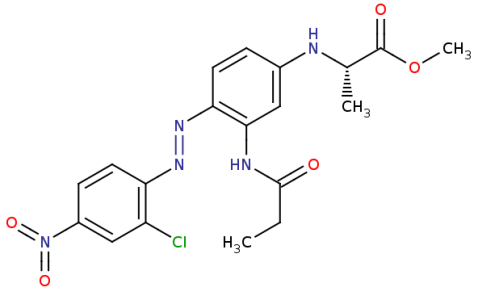
3164-29-2			EC number 221-618-9
52-89-1			EC number 200-157-7
657-27-2			EC number 211-519-9
172015-79-1			EC number 426-200-1

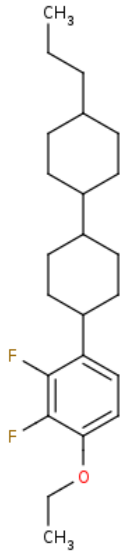
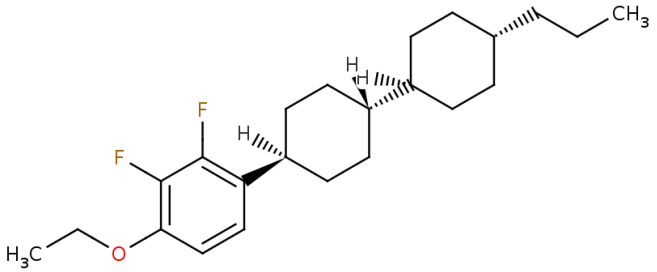
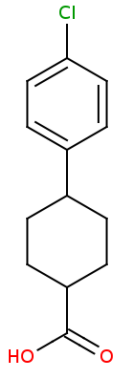
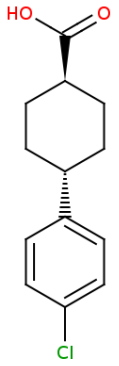
176380-53-3			EC number 439-410-3
6368-20-3			EC number 444-670-6
200509-41-7			EC number 414-200-4
13832-70-7 (incorrect)			EC number 419-580-5

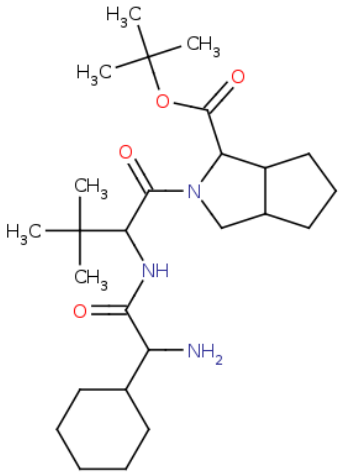
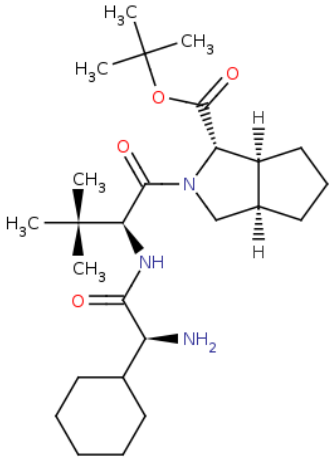
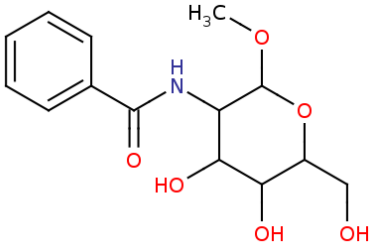
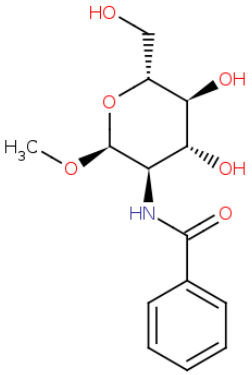
13832-70-7 (correct)			EC number 419-580-5
125224-62-6	 HBr HBr	 HBr HBr	EC number 411-000-9
129738-42-7			EC number 429-580-7

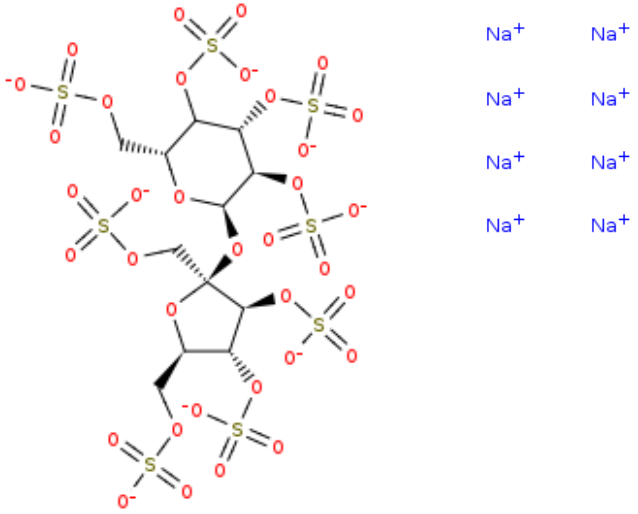
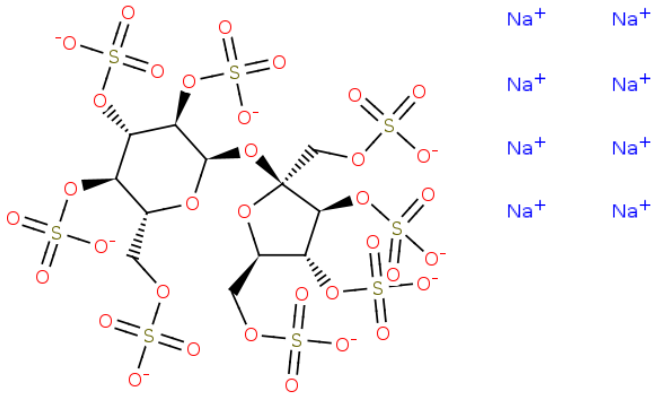
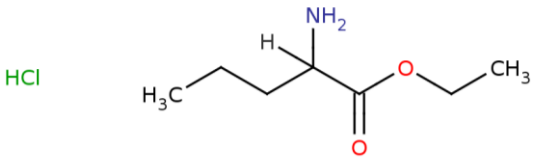
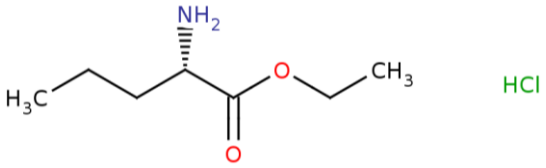
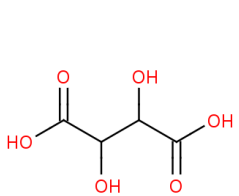
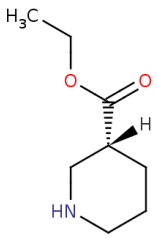
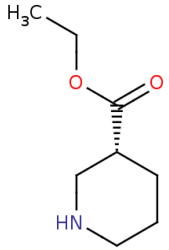
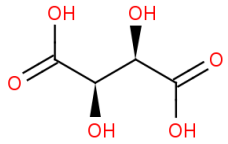
32981-86-5			EC number 418-680-6
31560-20-0			EC number 411-020-8
162537-11-3			EC number 431-620-3
478273-36-8			EC number 441-180-4

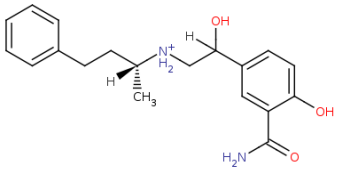
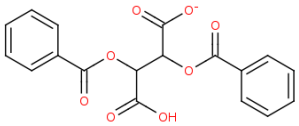
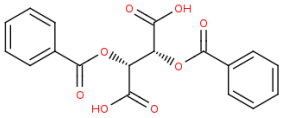
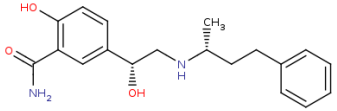
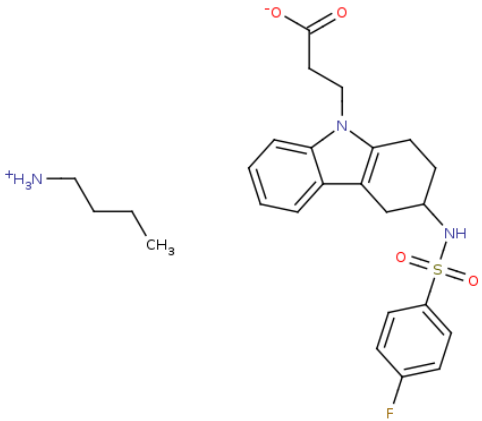
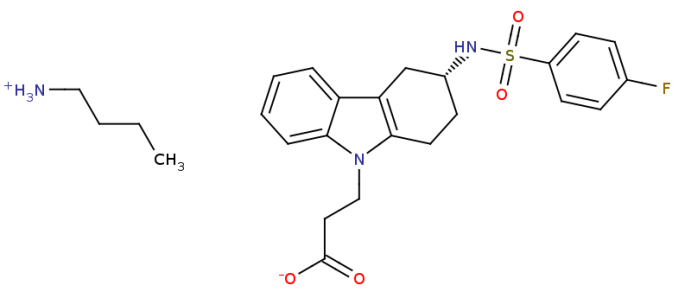
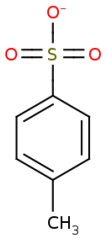
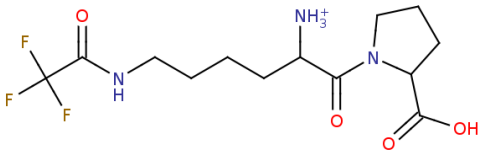
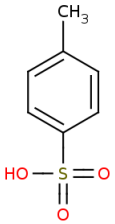
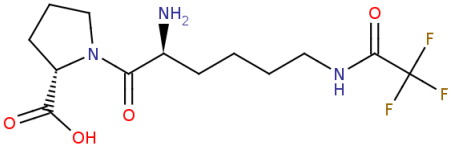
23477-67-0			EC number 419-120-3
124285-42-3			EC number 418-590-7
60166-91-8			EC number 410-940-7
103300-91-0			EC number 405-650-2

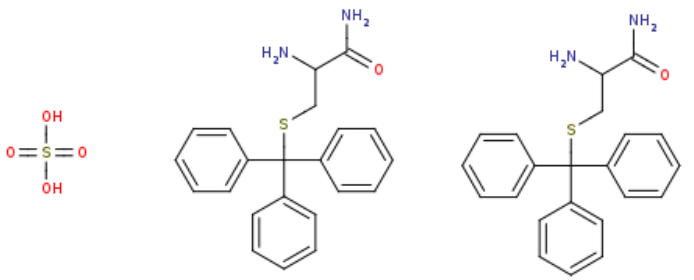
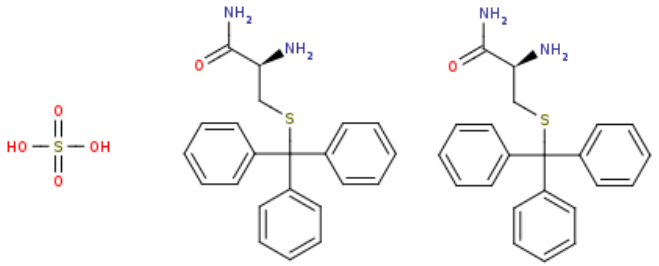
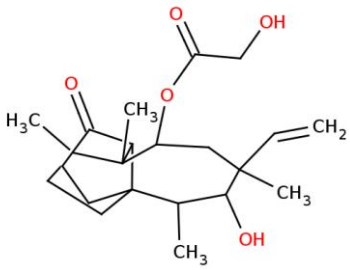
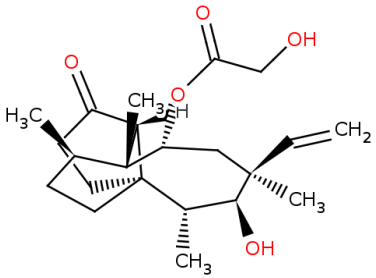
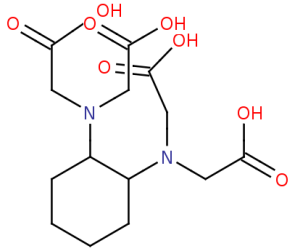
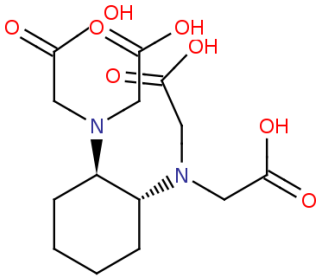
105351-42-6			EC number 806-827-0
155522-12-6			EC number 416-240-8

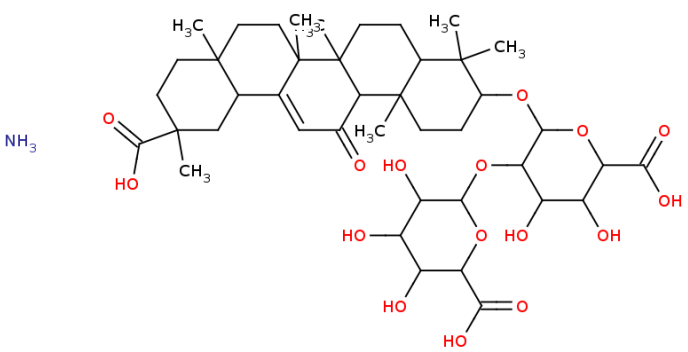
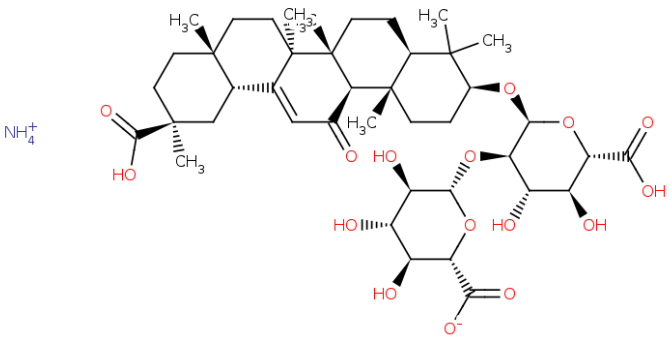
123560-48-5			EC number 602-941-8
49708-81-8			EC number 406-380-8

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

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

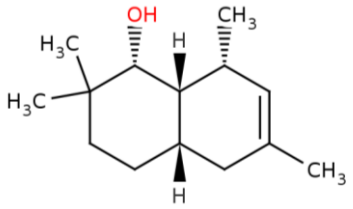
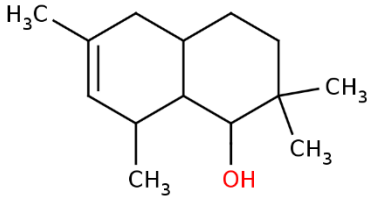
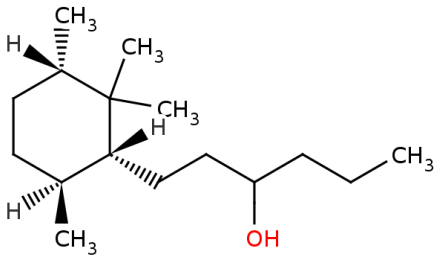
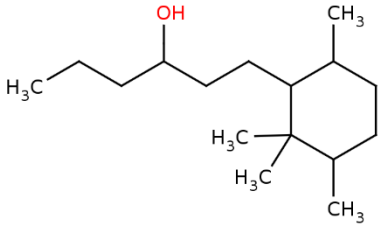
88976-55-0	 	 	EC number 404-390-7
1182723-73-4			EC number 925-462-9
105641-23-4	 	 	EC number 402-160-0

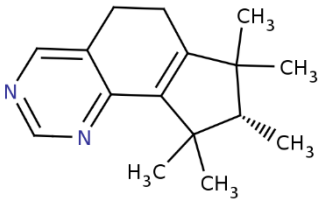
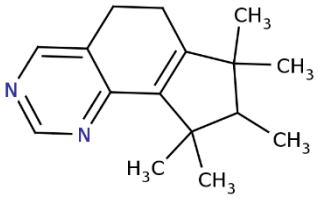
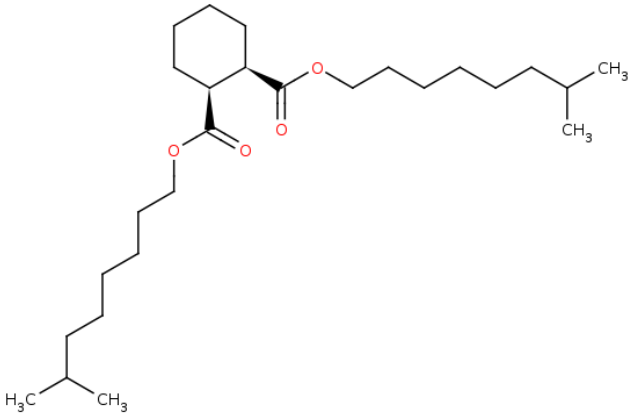
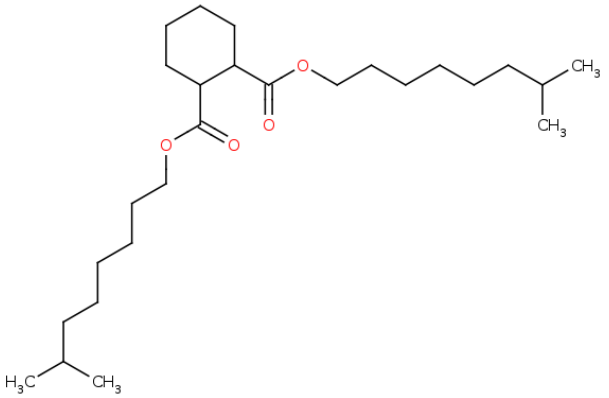
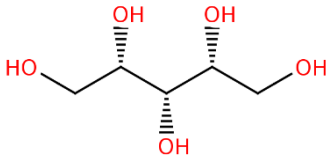
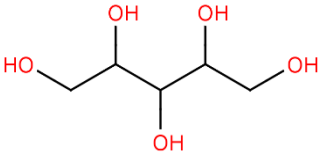
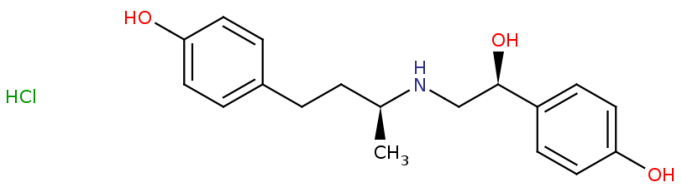
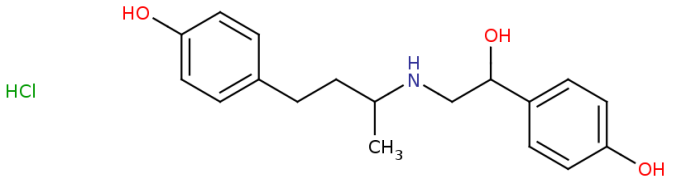
166737-86-6			EC number 429-450-1
125-65-5			EC number 204-747-5
13291-61-7			EC number 236-308-9

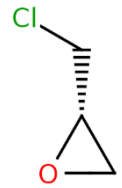
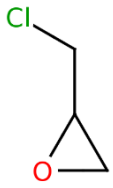
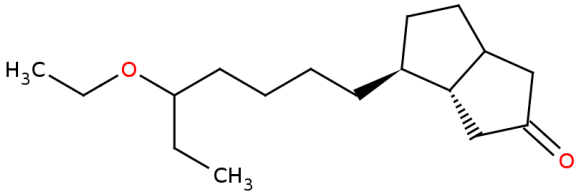
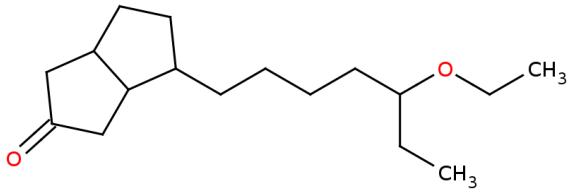
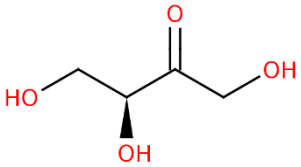
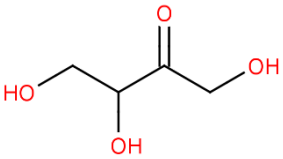
53956-04-0			EC number 258-887-7

7) Inconsistencies related to the stereochemistry (available stereochemistry information in the ECHA database were SciFinder^n has none)

Table 7: 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 available stereochemistry information in the ECHA database were SciFinder^n has none.

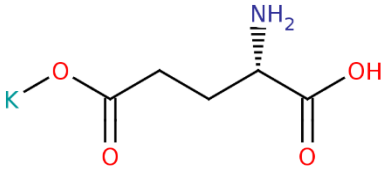
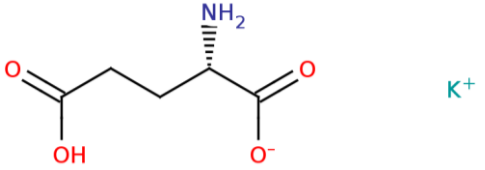
CAS RN™	Structure in the database	Structure corresponding to the CAS RN™	Comment
103614-86-4			EC number 434-960-0
95851-08-4			EC number 478-330-3

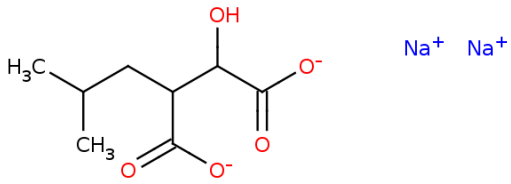
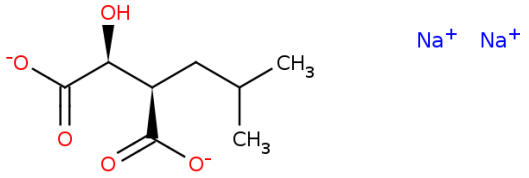
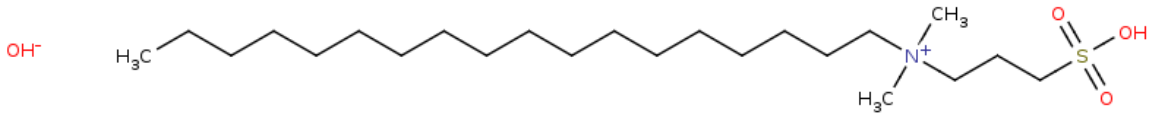
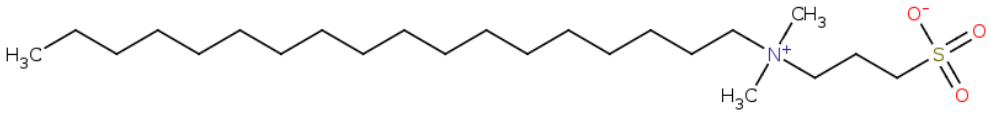
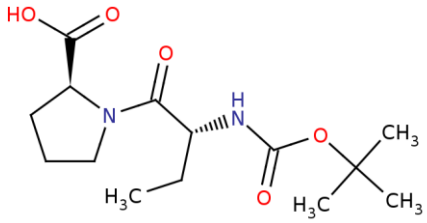
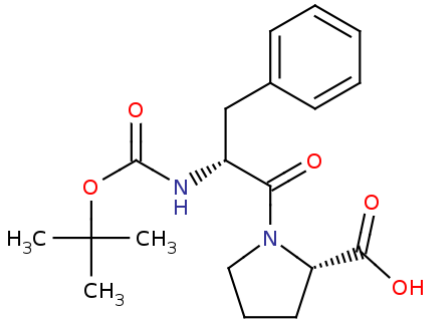
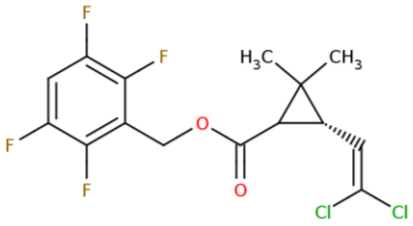
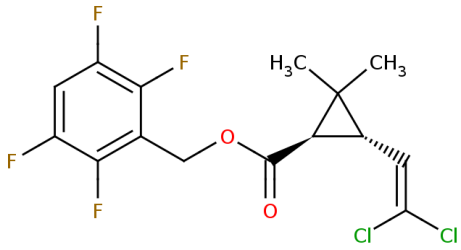
1315251-11-6			EC number 801-093-8
166412-78-8			EC number 431-890-2
87-99-0			EC number 201-788-0
90274-24-1			EC number 415-170-5

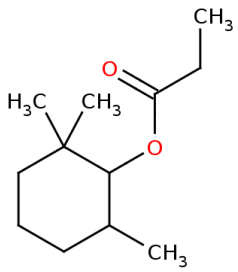
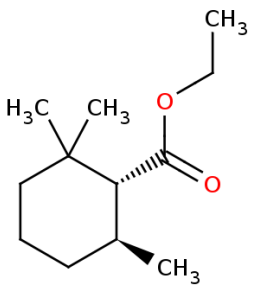
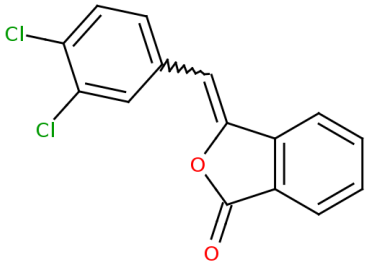
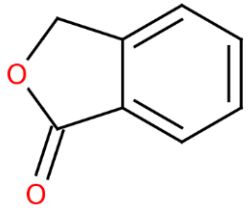
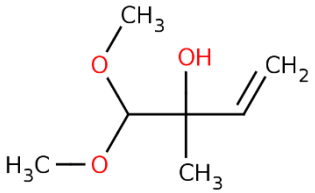
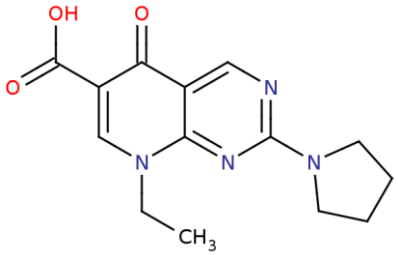
106-89-8			EC number 482-080-0
99778-68-4			EC number 419-880-6
40031-31-0			EC number 443-800-9

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			EC number 412-540-8
87-41-2			EC number 417-930-1
19562-30-2			EC number 419-730-1