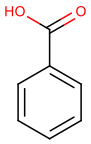
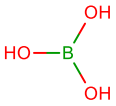
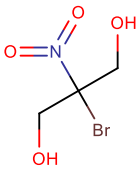
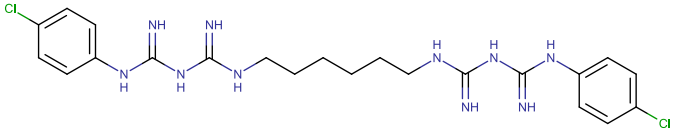
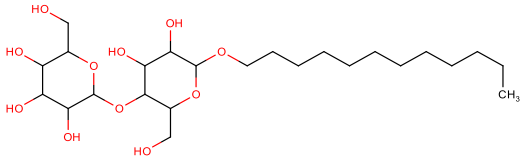
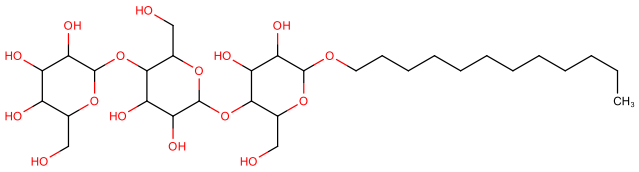
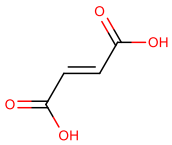
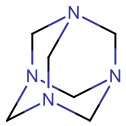
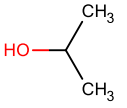
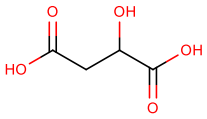
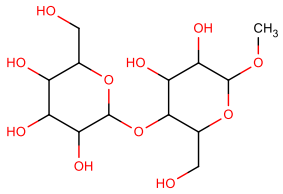
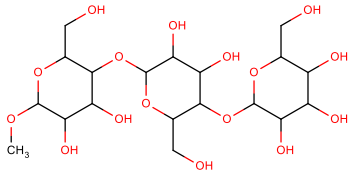
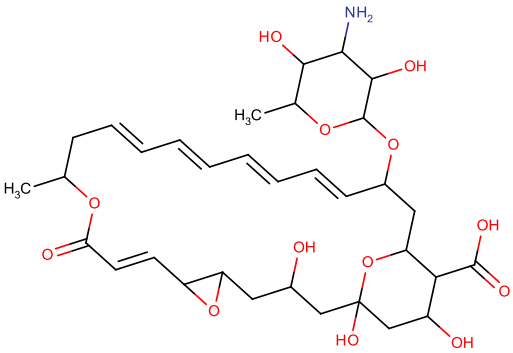
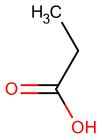
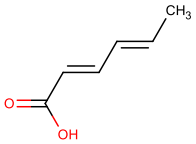
Annex Table III. Possible substitutive compound for parabens P1_S and P2_S (methyl paraben and ethyl paraben) considering a series of preservatives suitable for cosmetics, food, cleaning products and pharmaceuticals.

ID	CAS N°	Chemical name, synonims	SMILES	Structure
P1	65-85-0	Benzoic acid	OC(=O)C1=CC=CC=C1	
P2	10043-35-3	Boric acid	OB(O)O	
P3	52-51-7	Bronopol	OCC(Br)(CO)N(=O)=O	
P4	55-56-1	Chlorexidine	Clc1ccc(NC(=N)NC(=N)NCCCCCCNC(=N)NC(=N)Nc2ccc(Cl)cc2)cc1	
P5	69227-93-6	Dodecyl maltoside; dodecyl-β-D-maltoside; DoG2	OCC2OC(OC1C(O)C(O)C(O(CCCCCCCCCCCC))OC1(CO))C(O)C(O)C2(O)	
P6		Dodecyl maltotrioside; dodecyl-β-D-maltotrioside; DoG3	OCC1OC(OC2C(O)C(O)C(OC3C(O)C(O)C(O(CCCCCCCCCCCC))OC3CO)OC2CO)C(O)C(O)C1O	
P7	110-17-8	Fumaric acid	OC(=O)\C=C\C(O)=O	
P8	100-97-0	Hexamethylenetetramine	C1N2CN3CN1CN(C2)C3	
P9	67-63-0	Isopropil Alcohool	CC(C)O	

P10	6915-15-7	Malic acid	OC(CC(O)=O)C(O)=O	
P11	744-05-8	Methyl maltoside; methyl-β-D-maltoside; MeG2	OCC2OC(OC1C(O)C(O)C(O(C))OC1(CO))C(O)C(O)C2(O)	
P12		Methyl maltotrioside; methyl-β-D-maltotrioside; MeG3	OCC1OC(OC2C(O)C(O)C(OC3C(O)C(O)C(O(C))OC3CO)OC2CO)C(O)C(O)C1O	
P13	7681-93-8	Natamycin	C[CH]1O[CH](O[CH]2C[CH]3O[C](O)(C[CH](O)[CH]3C(O)=O)C[CH](O)C[CH]3O[CH]3\C=C\C(=O)O[CH](C)C\C=C\C=C\C=C\C=C\2)[CH](O)[CH](N)[CH]1O	
P14	79-09-4	Propionic acid	CCC(O)=O	
P15	110-44-1	Sorbic acid	C\C=C\C=C\C(O)=O	
P16	3380-34-5	Triclosan	OC1=CC(Cl)=CC=C1OC1=CC=C(Cl)C=C1Cl