Supporting Information

Metal-Organic Frameworks for Food Safety

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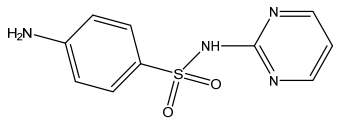
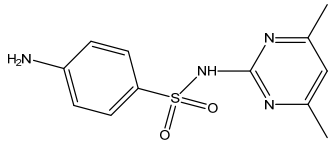
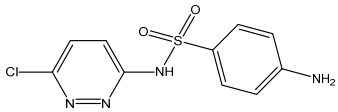
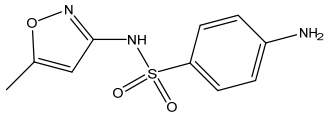
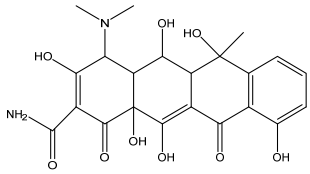
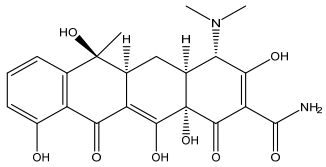
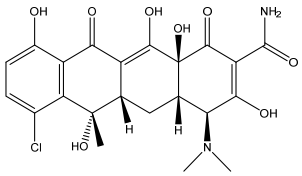
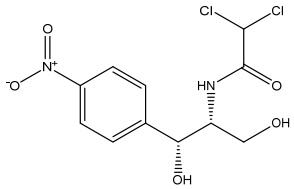
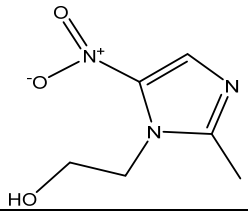
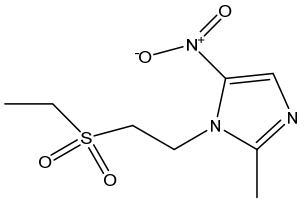
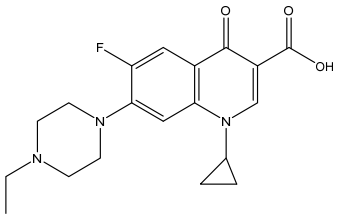
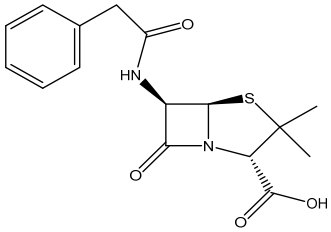
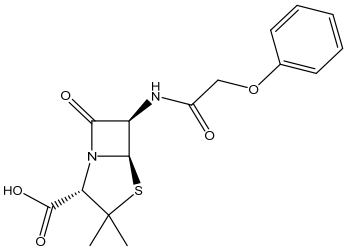
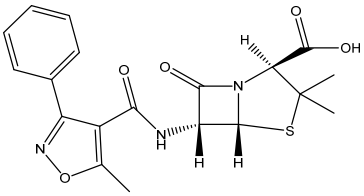
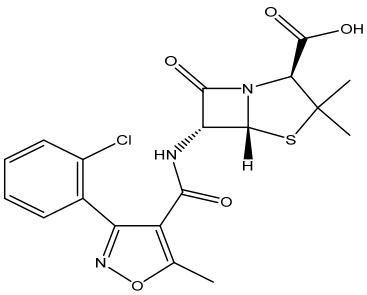
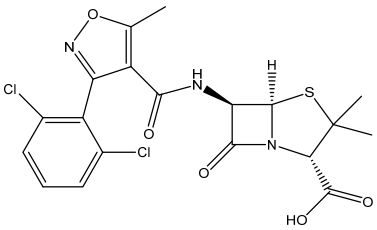
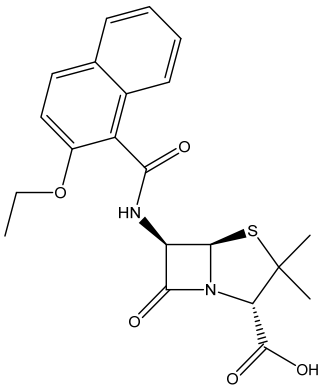
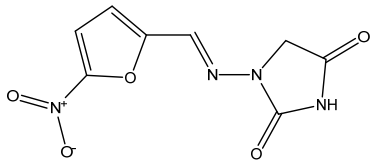
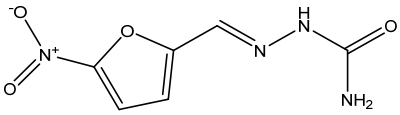
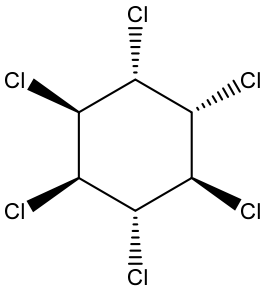
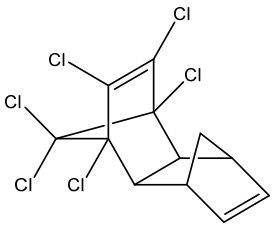
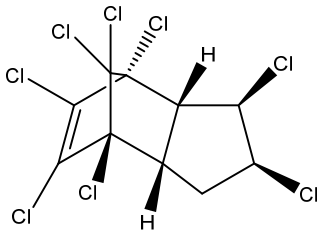
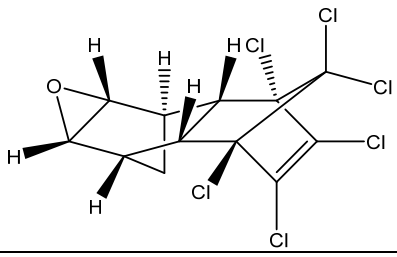
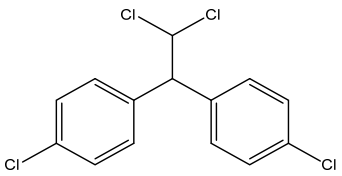
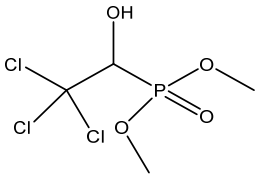
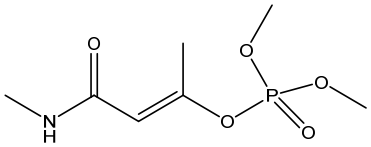
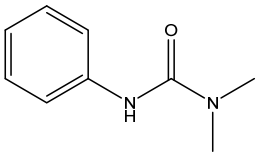
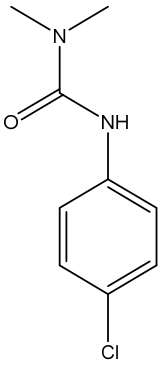
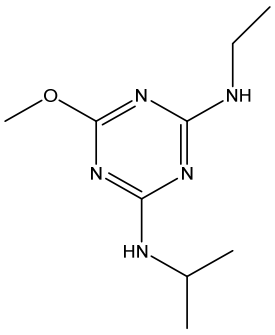
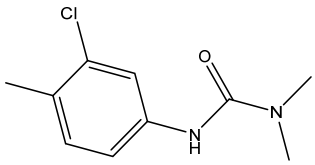
Appendix

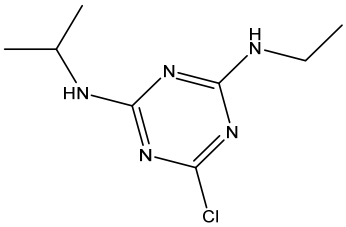
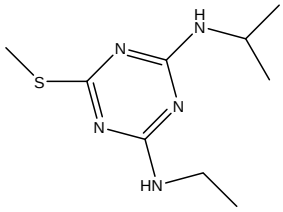
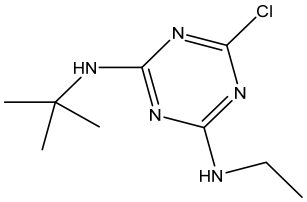
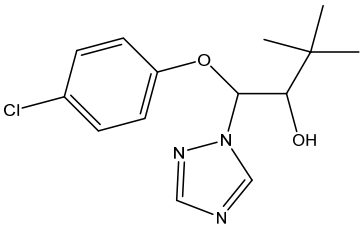
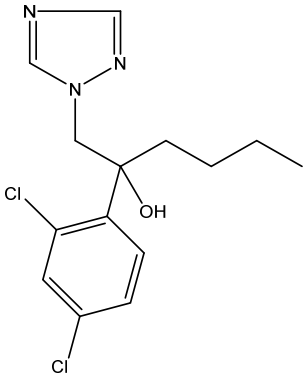
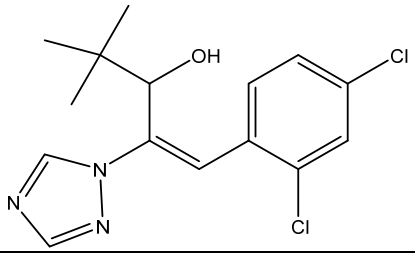
The molecular structures of typical compounds affecting food safety (mostly discussed in this review).

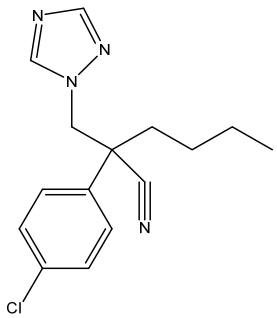
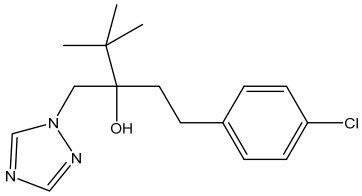
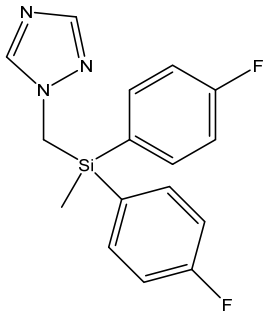
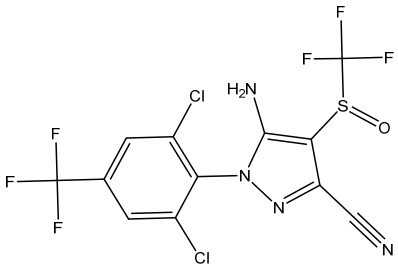
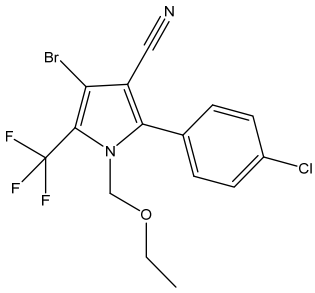
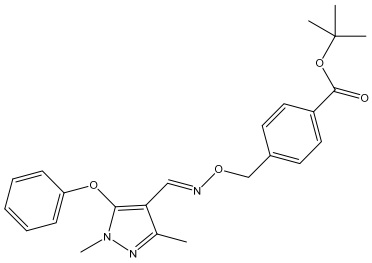
Target analytes	Formula	Molecular structure
Veterinary compounds		
Sulfadiazine	$C_{10}H_{10}N_4O_2S$	
Sulfamethazine	$C_{12}H_{14}N_4O_2S$	
Sulfachloropyridazine	$C_{10}H_9ClN_4O_2S$	
Sulfamethoxazole	$C_{10}H_{11}N_3O_3S$	
Oxytetracycline	$C_{22}H_{24}N_2O_9$	
Tetracycline	$C_{22}H_{24}N_2O_8$	
Chlorotetracycline	$C_{22}H_{23}ClN_2O_8$	
Chloramphenicol	$C_{11}H_{12}Cl_2N_2O_5$	
Metronidazole	$C_6H_9N_3O_3$	

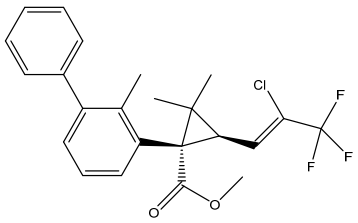
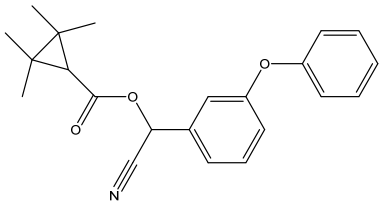
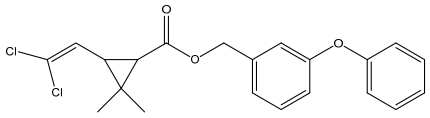
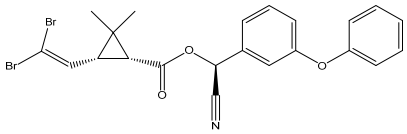
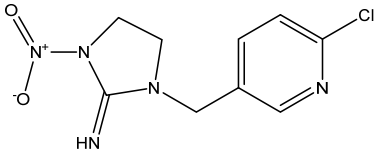
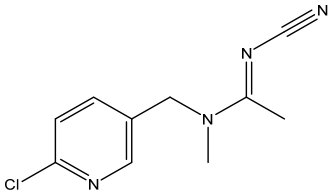
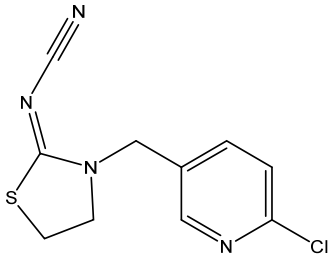
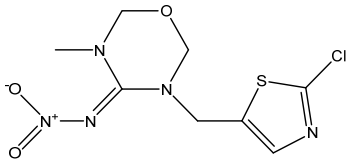
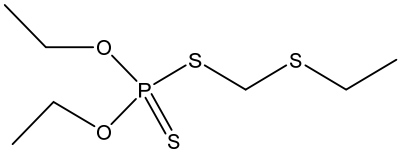
Tinidazole	$C_8H_{13}N_3O_4S$	
Enrofloxacin	$C_{19}H_{22}FN_3O_3$	
Penicillin G	$C_{16}H_{18}N_2O_4S$	
Penicillin V	$C_{16}H_{18}N_2O_5S$	
Oxacillin	$C_{19}H_{19}N_3O_5S$	
Cloxacillin	$C_{19}H_{18}ClN_3O_5S$	
Dicloxacillin	$C_{19}H_{17}Cl_2N_3O_5S$	

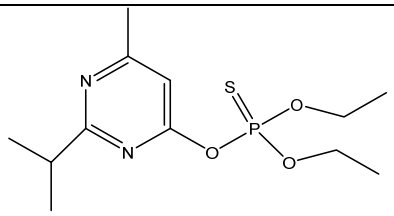
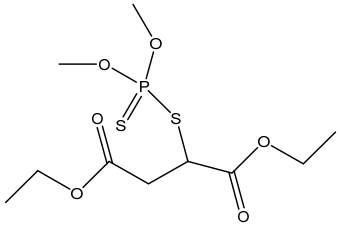
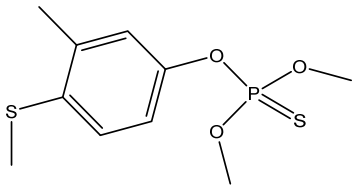
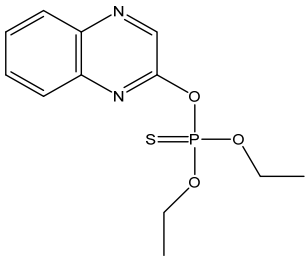
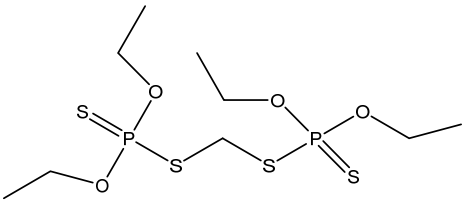
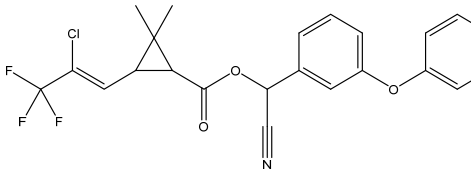
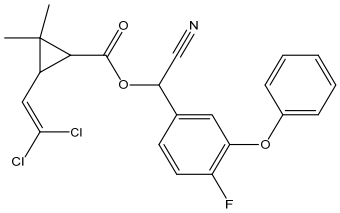
Nafcillin	$C_{21}H_{22}N_2O_5S$	
Nitrofurantoin	$C_8H_6N_4O_5$	
Nitrofurazone	$C_6H_6N_4O_4$	
Pesticide residues		
α-HCH	$C_6H_6Cl_6$	
Aldrin	$C_{12}H_8Cl_6$	
α-chlordane	$C_{10}H_6Cl_8$	
Dieldrin	$C_{12}H_8Cl_6O$	

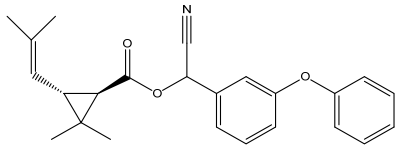
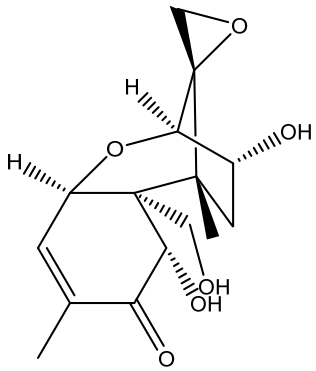
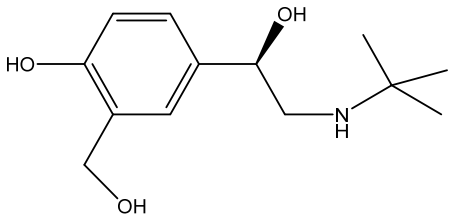
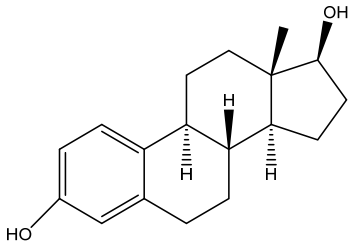
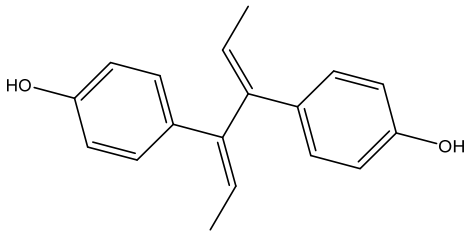
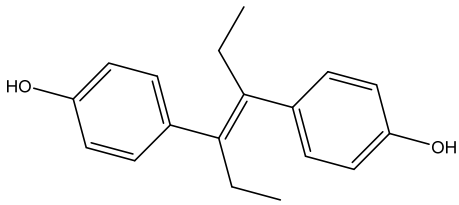
p,p'-DDD	$C_{14}H_{10}Cl_4$	
Trichlorfon	$C_4H_8Cl_3O_4P$	
Monocrotophos	$C_7H_{14}NO_5P$	
Fenuron	$C_9H_{12}N_2O$	
Monuron	$C_9H_{11}ClN_2O$	
Atraton	$C_9H_{17}N_5O$	
Chlorotoluron	$C_{10}H_{13}ClN_2O$	

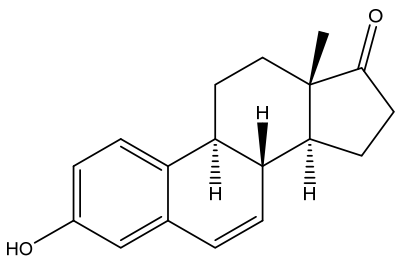
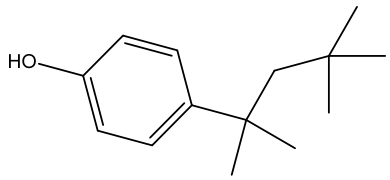
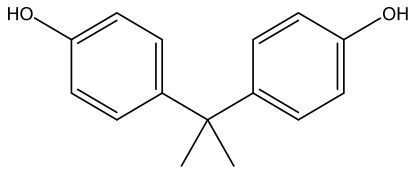
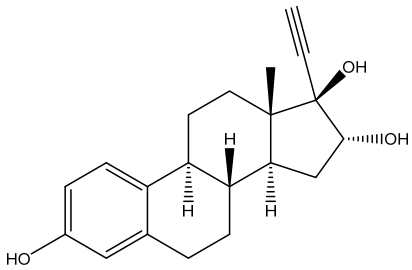
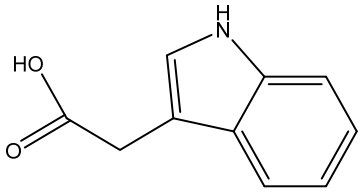
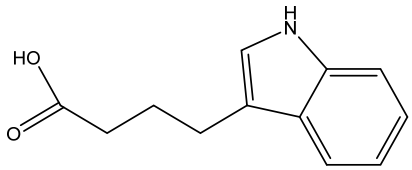
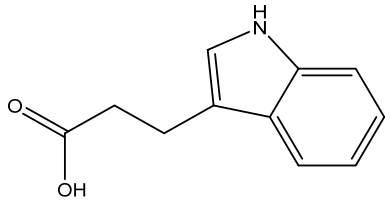
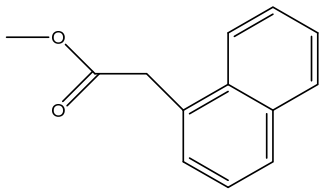
Atrazine	$C_8H_{14}ClN_5$	
Ametryn	$C_9H_{17}N_5S$	
Terbuthylazine	$C_9H_{16}ClN_5$	
Triadimenol	$C_{14}H_{18}ClN_3O_2$	
Hexaconazole	$C_{14}H_{17}Cl_2N_3O$	
Diniconazole	$C_{15}H_{17}Cl_2N_3O$	

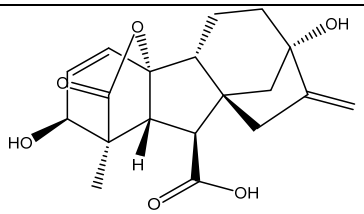
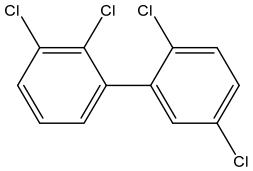
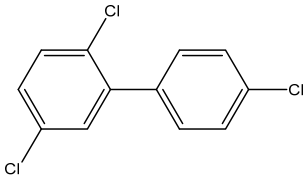
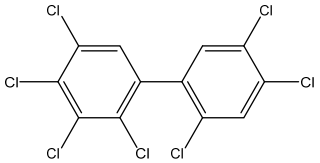
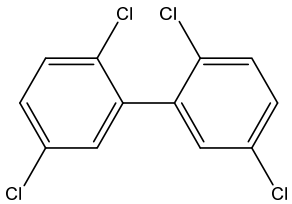
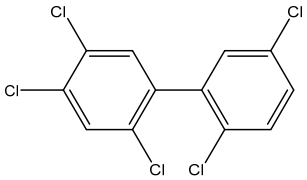
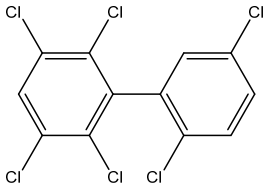
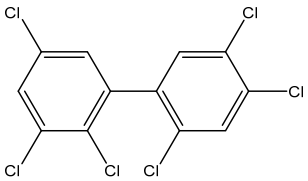
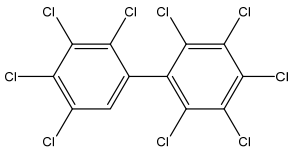
Myclobutanil	$C_{15}H_{17}ClN_4$	
Tebuconazole	$C_{16}H_{22}ClN_3O$	
Flusilazole	$C_{16}H_{15}F_2N_3Si$	
Fipronil	$C_{12}H_4Cl_2F_6N_4OS$	
Chlorfenapyr	$C_{15}H_{11}BrClF_3N_2O$	
Fenpyroximate	$C_{24}H_{27}N_3O_4$	

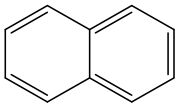
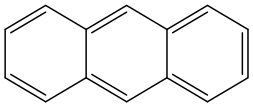
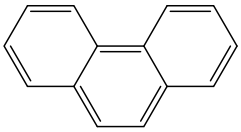
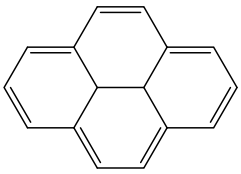
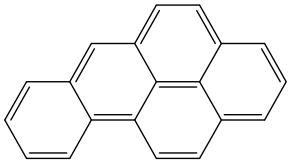
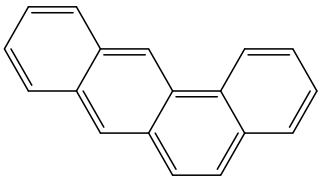
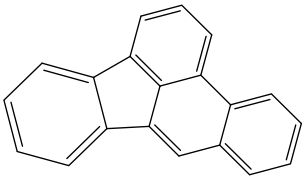
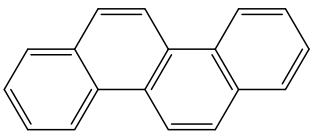
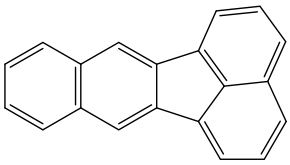
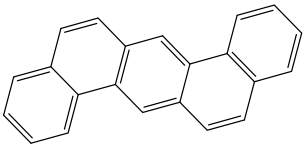
Bifenthrin	$C_{23}H_{22}ClF_3O_2$	
Fenpropathrin	$C_{22}H_{23}NO_3$	
Permethrin	$C_{21}H_{20}Cl_2O_3$	
Deltamethrin	$C_{22}H_{19}Br_2NO_3$	
Imidacloprid	$C_9H_{10}ClN_5O_2$	
Acetamiprid	$C_{10}H_{11}ClN_4$	
Thiacloprid	$C_{10}H_9ClN_4S$	
Thiamethoxam	$C_8H_{10}ClN_5O_3S$	
Phorate	$C_7H_{17}O_2PS_3$	

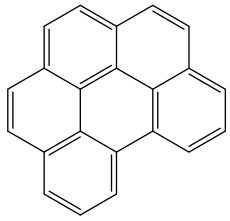
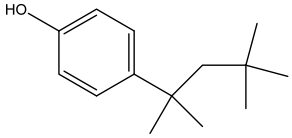
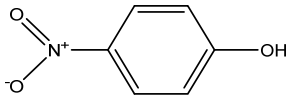
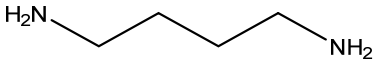
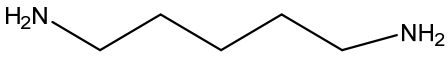
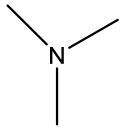
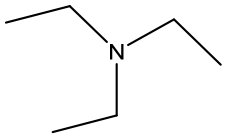
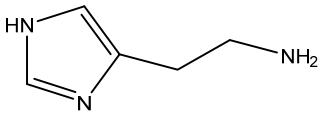
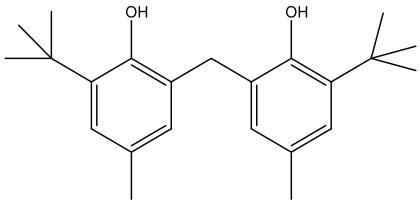
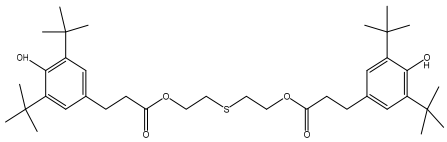
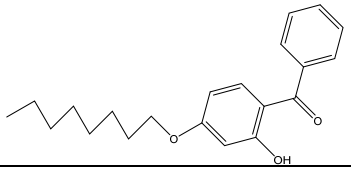
Diazinon	$C_{12}H_{21}N_2O_3PS$	
Malathion	$C_{10}H_{19}O_6PS_2$	
Fenthion	$C_{10}H_{15}O_3PS_2$	
Quinalphos	$C_{12}H_{15}N_2O_3PS$	
Ethion	$C_9H_{22}O_4P_2S_4$	
Cyhalothrin	$C_{23}H_{19}ClF_3NO_3$	
Beta-cyfluthrin	$C_{22}H_{18}Cl_2FNO_3$	

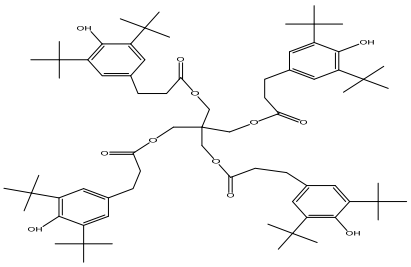
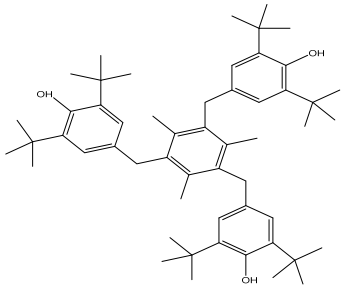
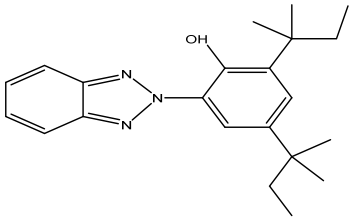
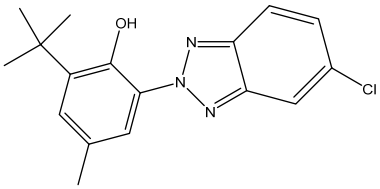
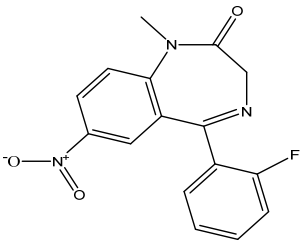
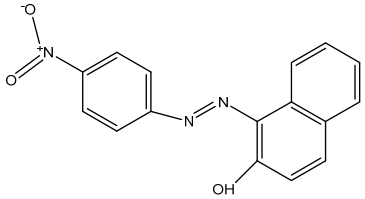
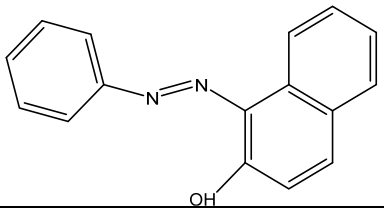
Cyphenothrin	$C_{24}H_{25}NO_3$	
Vomitoxin	$C_{15}H_{20}O_6$	
Salbutamol	$C_{13}H_{21}NO_3$	
Hormones		
17-β-estradiol (E2)	$C_{18}H_{24}O_2$	
Dienestrol	$C_{18}H_{18}O_2$	
Diethylstilbestrol	$C_{18}H_{20}O_2$	

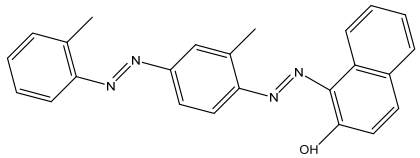
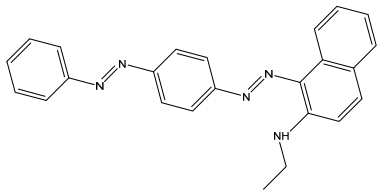
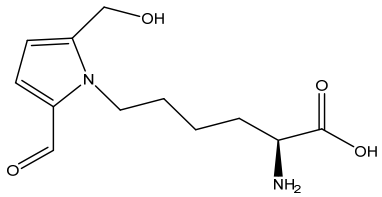
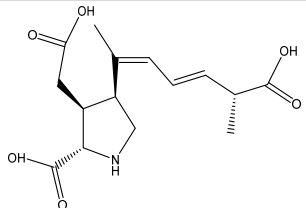
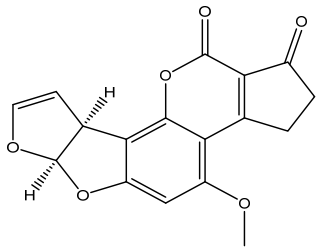
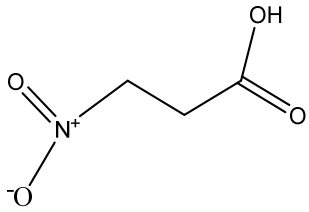
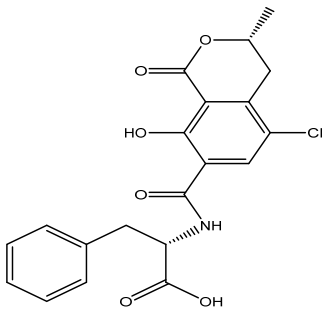
Estrone	$C_{18}H_{22}O_2$	
4-t-octylphenol	$C_{14}H_{22}O$	
Bisphenol-A	$C_{15}H_{16}O_2$	
17α-ethynylestradiol	$C_{20}H_{24}O_3$	
Indole-3-acetic acid	$C_{10}H_9NO_2$	
Indole-3-butyric acid	$C_{12}H_{13}NO_2$	
Indole-3-propionic acid	$C_{11}H_{11}NO_2$	
1-naphthaleneacetic	$C_{13}H_{12}O_2$	

Gibberellic acid	$C_{19}H_{22}O_6$	
PCB44	$C_{12}H_6Cl_4$	
PCB31	$C_{12}H_7Cl_3$	
PCB180	$C_{12}H_3Cl_7$	
PCB52	$C_{12}H_6Cl_4$	
PCB101	$C_{12}H_5Cl_5$	
PCB151	$C_{12}H_4Cl_6$	
PCB141	$C_{12}H_4Cl_6$	
PCB206	$C_{12}HCl_9$	

Naphthalene	$C_{10}H_8$	
Anthracene	$C_{14}H_{10}$	
Phenanthrene	$C_{14}H_{10}$	
Pyrene	$C_{16}H_{10}$	
Benzo[a]pyrene	$C_{20}H_{12}$	
Benzo[a]anthracene	$C_{18}H_{12}$	
Benzo[b]fluoranthene	$C_{20}H_{12}$	
Chrysene	$C_{18}H_{12}$	
Benzo[k]fluoranthene	$C_{20}H_{12}$	
Dibenzo[a,h]-anthracene	$C_{22}H_{14}$	

Benzo[ghi]perylene	$C_{22}H_{12}$	
4-tert-octylphenol	$C_{14}H_{22}O$	
4-nitrophenol	$C_6H_5NO_3$	
Organic amine		
Putrescine	$C_4H_{12}N_2$	
Cadaverine	$C_5H_{14}N_2$	
Trimethylamine	C_3H_9N	
Triethylamine	$C_6H_{15}N$	
Histamine	$C_5H_9N_3$	
Additives and dyes		
Cyanox 2246	$C_{23}H_{32}O_2$	
Irganox 1035	$C_{38}H_{58}O_6S$	
Chimassorb 81	$C_{21}H_{26}O_3$	

Irganox 1010	$C_{73}H_{108}O_{12}$	
Irganox 1330	$C_{54}H_{78}O_3$	
Tinuvin 328	$C_{22}H_{29}N_3O$	
Tinuvin 326	$C_{17}H_{18}ClN_3O$	
Flunitrazepam	$C_{16}H_{12}FN_3O_3$	
Para Red	$C_{16}H_{11}N_3O_3$	
Sudan I	$C_{16}H_{12}N_2O$	

Sudan IV	$C_{24}H_{20}N_4O$	
Sudan Red 7B	$C_{24}H_{21}N_5$	
Pyrraline	$C_{12}H_{18}N_2O_4$	
Toxins		
Domoic acid	$C_{15}H_{21}NO_6$	
Aflatoxin B1	$C_{17}H_{12}O_6$	
3-nitropropionic acid	$C_3H_5NO_4$	
Ochratoxin A	$C_{20}H_{18}ClNO_6$