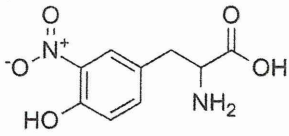
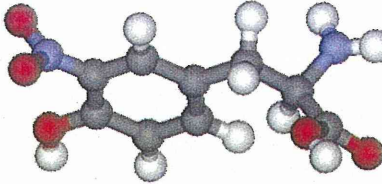
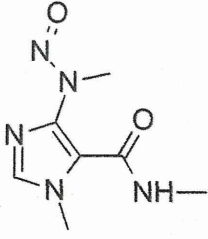
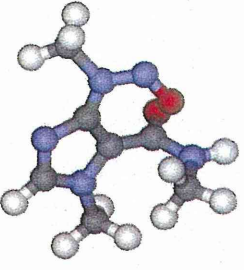
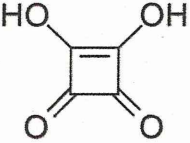
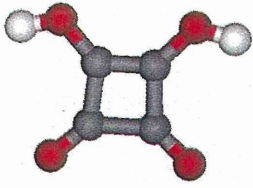
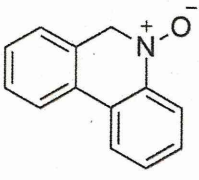
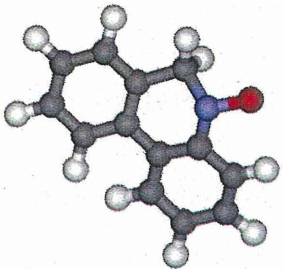
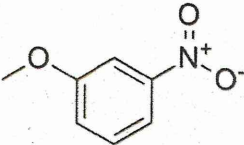
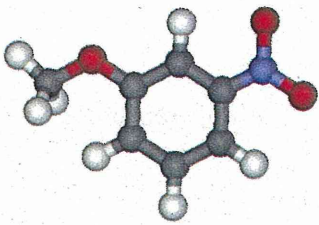
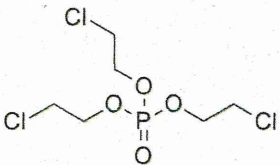
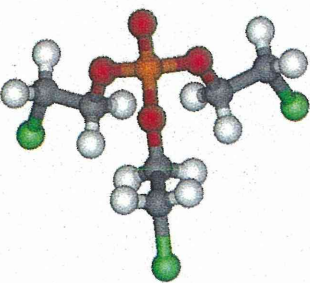
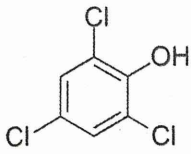
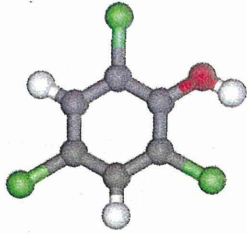
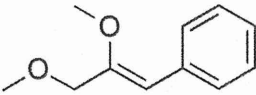
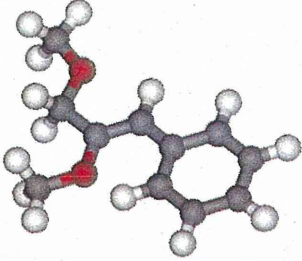
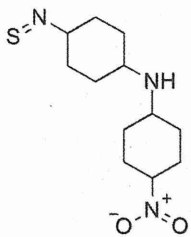
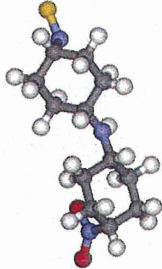
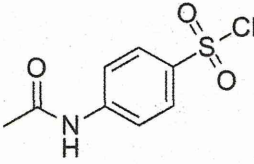
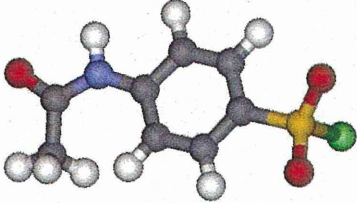
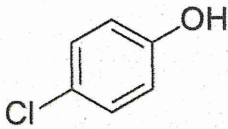
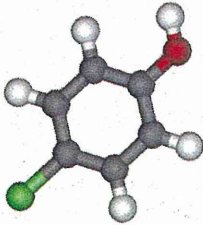
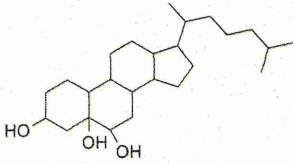
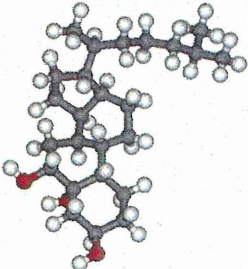
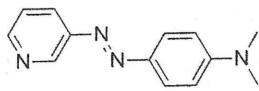
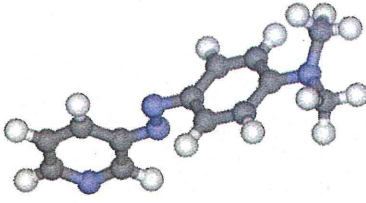
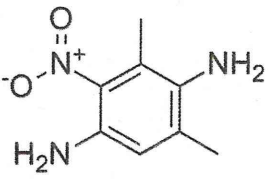
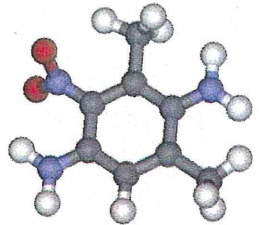
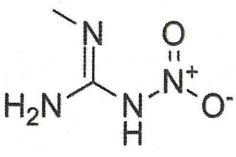
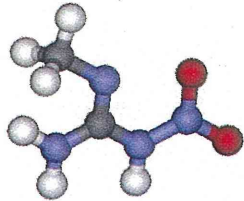
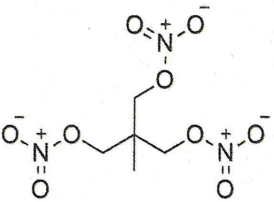
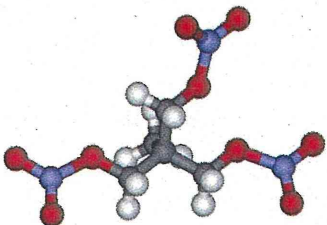
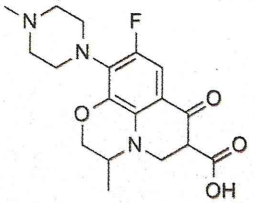
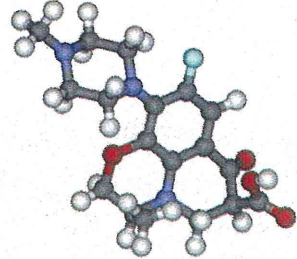
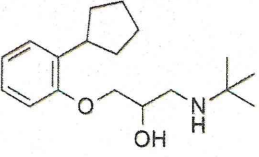
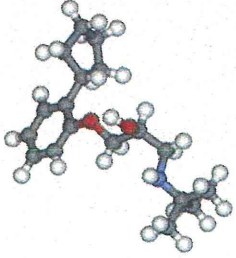
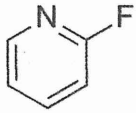
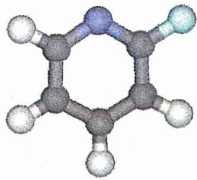
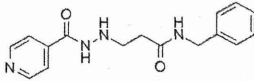
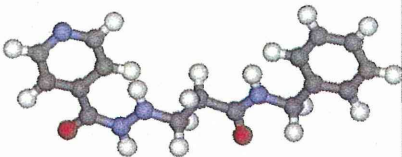
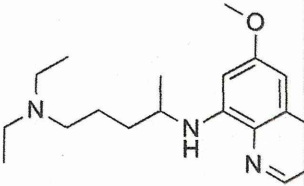
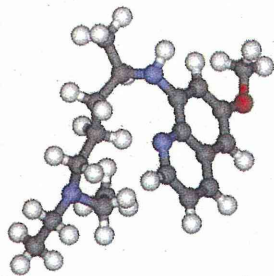
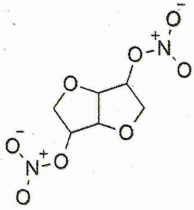
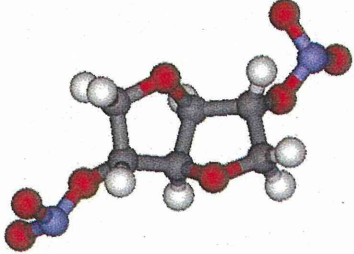
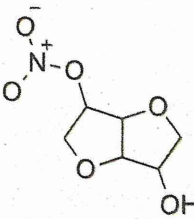
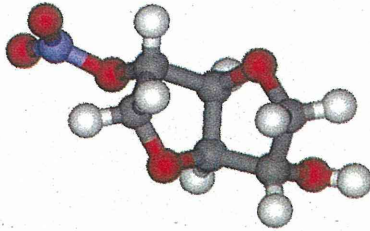
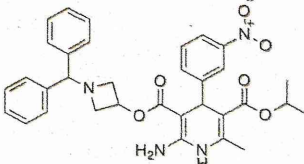
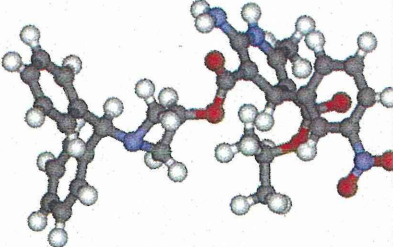
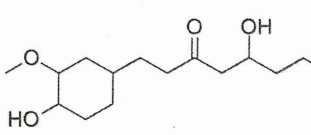
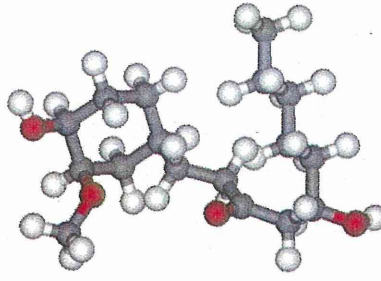
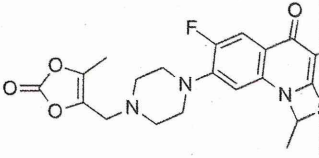
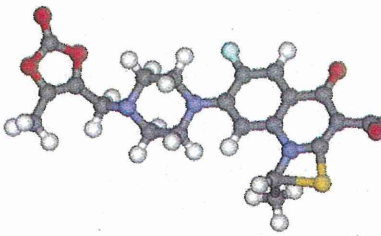
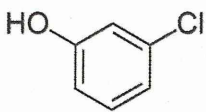
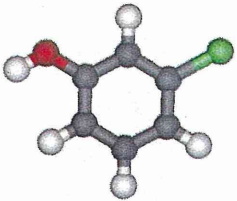
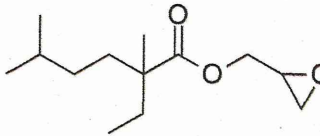
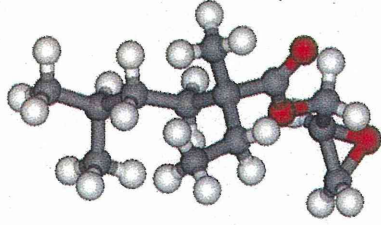
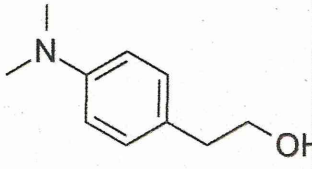
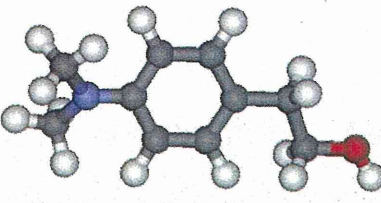
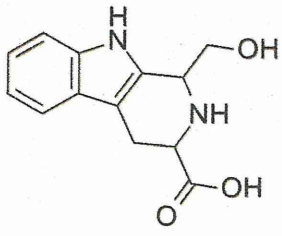
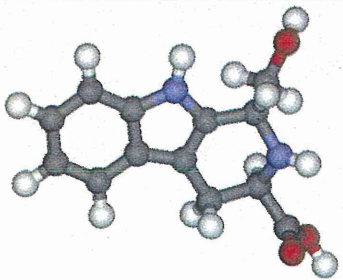


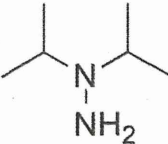
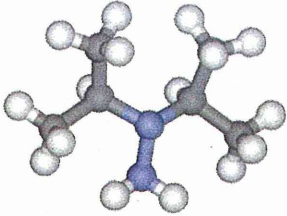
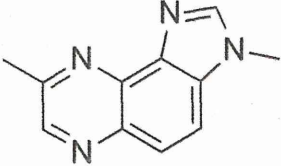
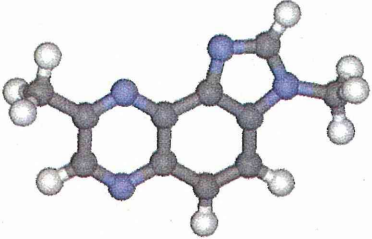
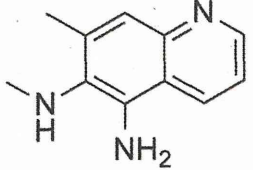
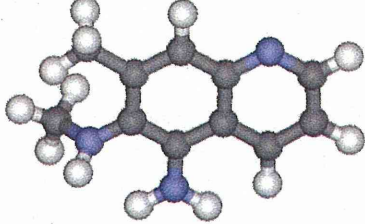

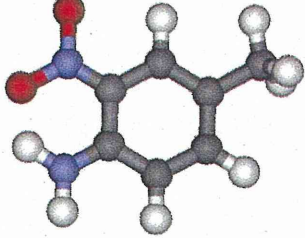
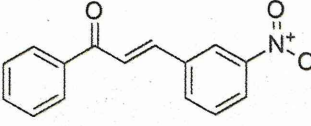
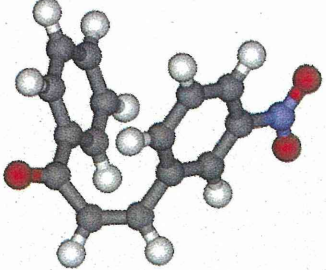
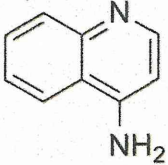
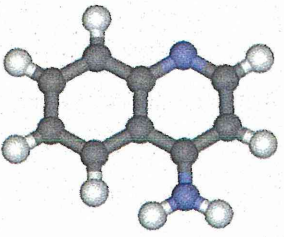
12	3-nitro-l-tyrosine		
13	mononitrosocaffeine		
14	3,4-dihydroxy-3-cyclobutene-1,2-dione		
15	2-nitrobiphenyl		
16	m-nitroanisole		
17	tris(chloroethyl)phosphate		

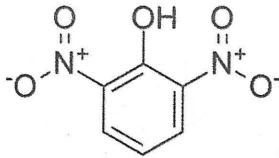
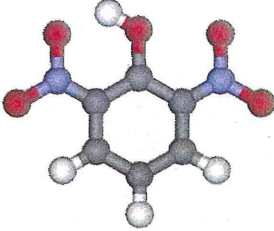
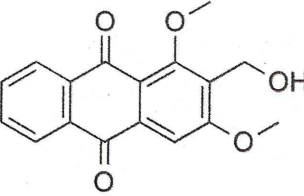
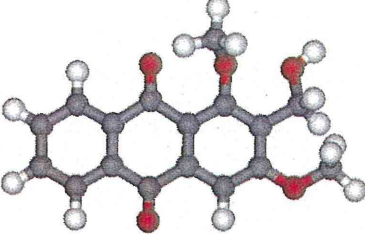
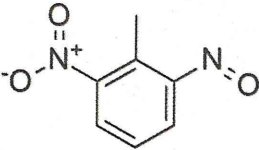
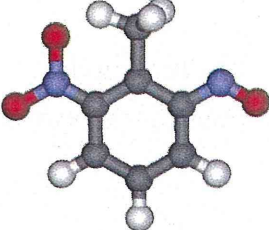
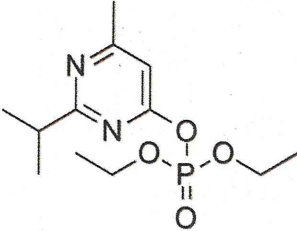
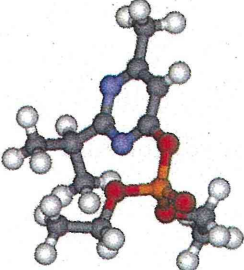
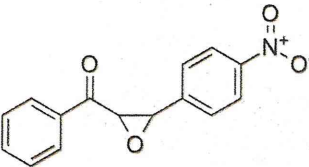
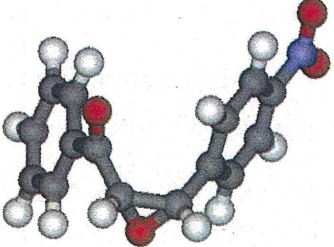
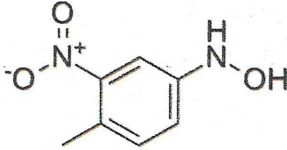
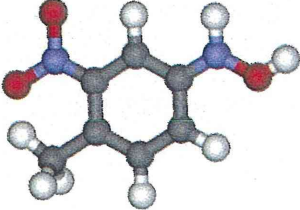
18	2,4,6-trichlorophenol		
19	z-2,3-dimethoxyprop-1-enylbenzene		
20	amoscanate		
21	4-(acetylamino)benzenesulfonyl chloride		
22	4-chlorophenol		
23	cholestane-3beta,5alpha,6beta-triol		

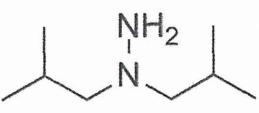
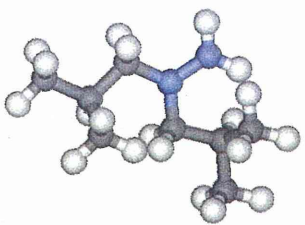
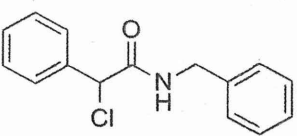
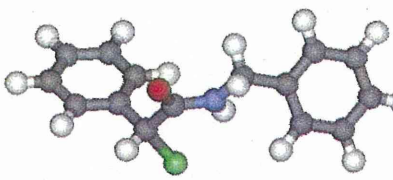
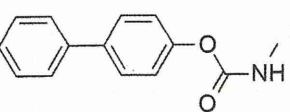
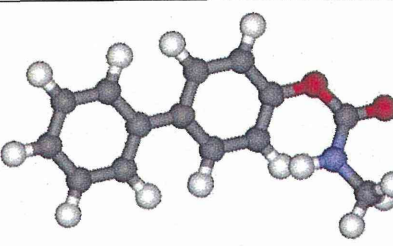
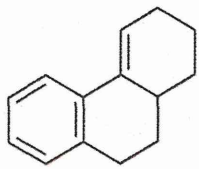
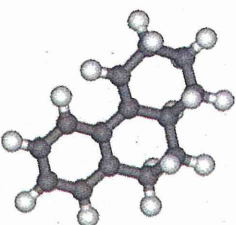
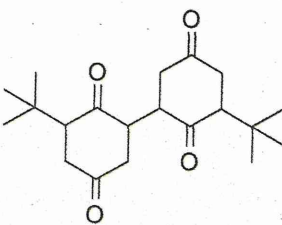
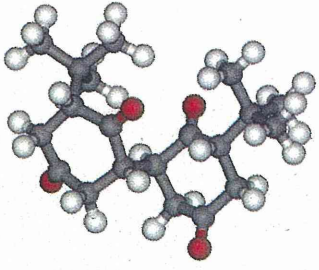
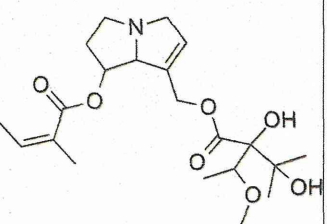
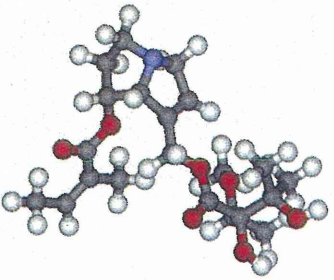
24	4'-(n,n-dimethylamino)-1'-phenylazo-3-pyridine		
25	4-amino-3-nitro-2,6-dimethylaniline		
26	n-methyl-n'-nitroguanidine		
27	trimethylolethane trinitrate		
28	dr3354		
29	(-)-penbutolol		

30	2-fluoropyridine		
31	nialamide		
32	pamaquine		
33	isodinit		
34	monisid		
35	azelnidipine		

36	gingerol		
37	prulifloxacin		
38	3-chlorophenol		
39	neodecanoic acid, 2,3-epoxypropyl ester		
40	4-(dimethylamino) benzeneethanol		
41	### tetrahydro-beta-carboline-3-carboxylic acid		

42	n,n-diisopropylhydrazine		
43	3,8-dimethyl-3h-imidazo[4,5-f]quinoxaline		
44	6,7-dimethylquinoline-5,6-diamine		
45	4-methyl-2-nitroaniline		
46	3-nitrochalcone		
47	4-aminoquinoline		

48	2,6-dinitrophenol		
49	2-(hydroxymethyl)-1,3-dimethoxyanthraquinone		
50	2-nitroso-6-nitrotoluene		
51	diazoxon		
52	4-nitrochalcone oxide		
53	4-hydroxylamino-2-nitrotoluene		

54	n,n-diisobutylhydrazine		
55	n-benzyl-2-chloro-2-phenylacetamide		
56	p-biphenyl n-methylcarbamate		
57	1,2,3,9,10,10a-hexahydrophenanthrene		
58	3,3'-di-tert-butylbiphenyldiquinone (2,5,2',5')		
59	lasiocarpine		

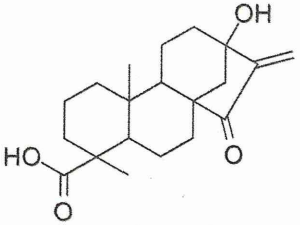
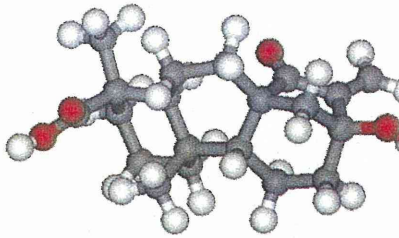
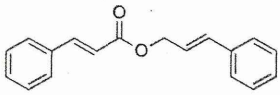
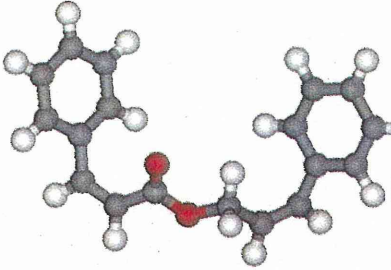
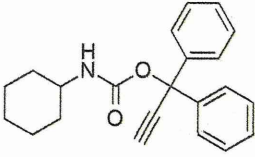
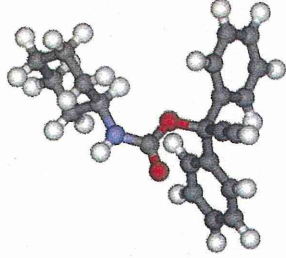
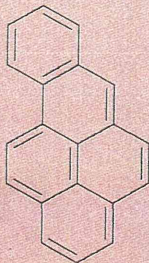
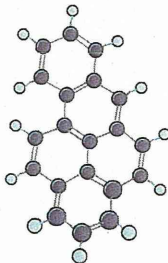

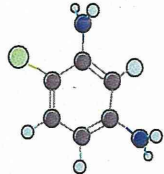
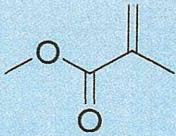
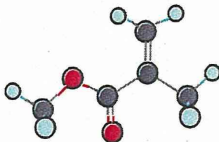
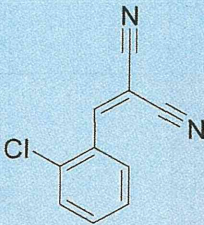
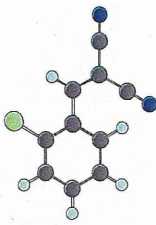

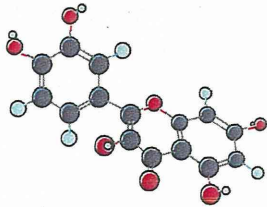
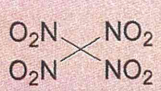
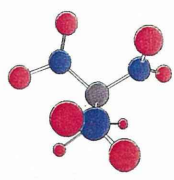
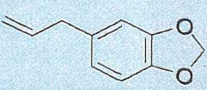
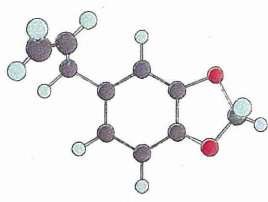
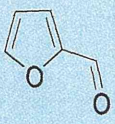
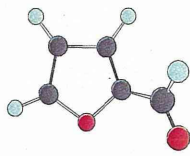
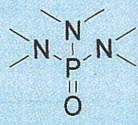
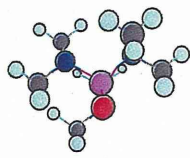

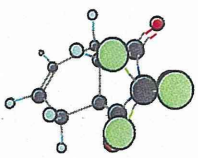
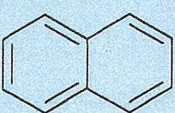
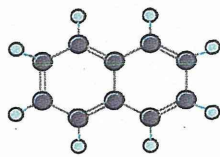
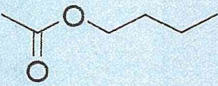
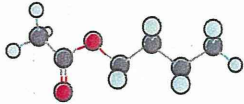
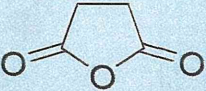
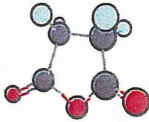

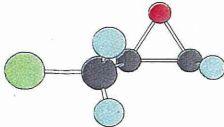

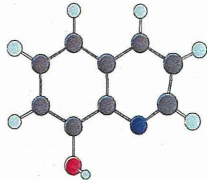
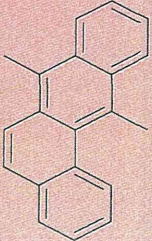
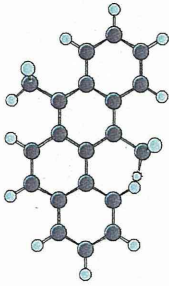
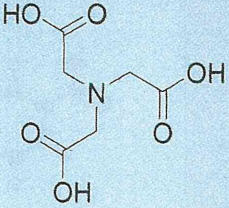
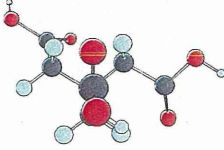
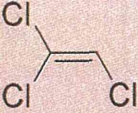
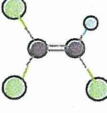
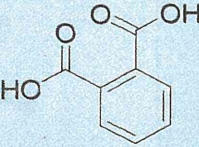
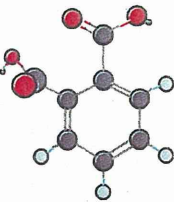
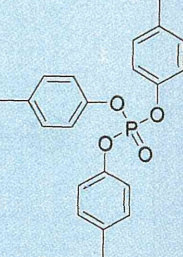
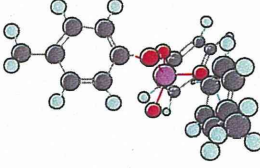
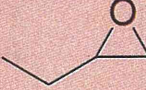
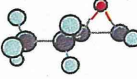
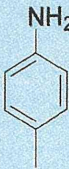
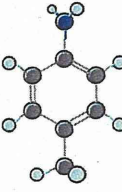
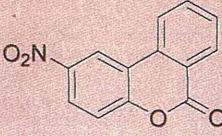
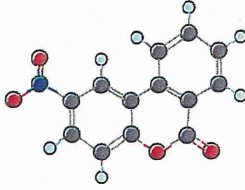
60	15-oxosteviol	 <p>Chemical structure of 15-oxosteviol, a complex steroid-like molecule with multiple fused rings, a hydroxyl group (OH), a carbonyl group (C=O), and a carboxylic acid group (HO-C=O).</p>	 <p>Ball-and-stick model of 15-oxosteviol, showing the spatial arrangement of atoms (carbon in grey, oxygen in red, hydrogen in white).</p>
61	cinnamyl cinnamate	 <p>Chemical structure of cinnamyl cinnamate, consisting of two cinnamyl groups linked by an ester bond.</p>	 <p>Ball-and-stick model of cinnamyl cinnamate, showing the spatial arrangement of atoms.</p>
62	1,1-diphenyl-2-propynyl-n-cyclohexyl carbamate	 <p>Chemical structure of 1,1-diphenyl-2-propynyl-n-cyclohexyl carbamate, featuring a cyclohexane ring attached to a carbamate group, which is further substituted with two phenyl rings and a propynyl group.</p>	 <p>Ball-and-stick model of 1,1-diphenyl-2-propynyl-n-cyclohexyl carbamate, showing the spatial arrangement of atoms, including the nitrogen atom in blue.</p>



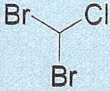

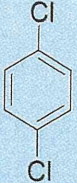
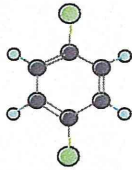
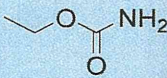
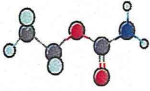
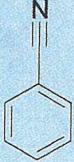
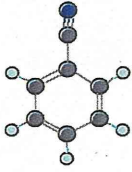
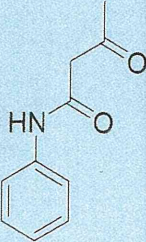
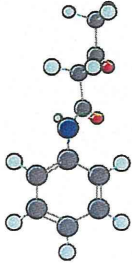
表 13 : 検証母集団の 214 化合物の最安定構造

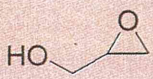
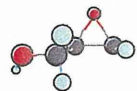
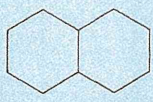
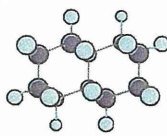
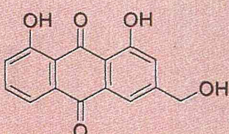
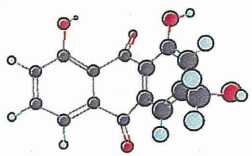


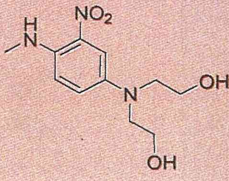
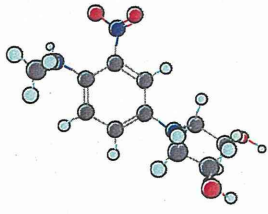
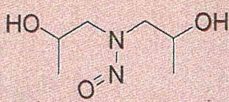
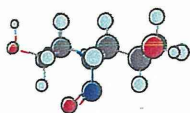
番号	化合物	3次元構造
1		
2		
3		
4		
5		


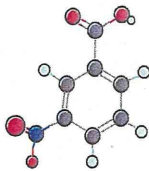
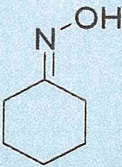
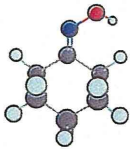
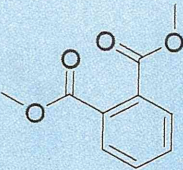
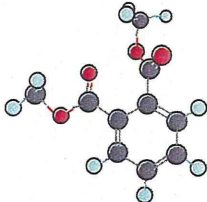
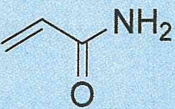
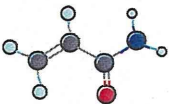
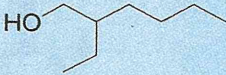
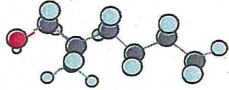
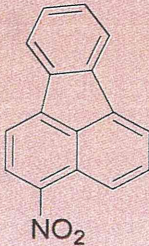
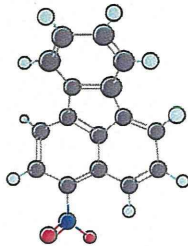
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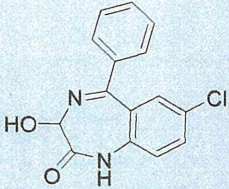
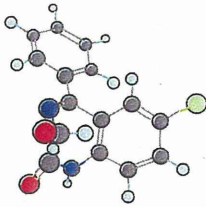
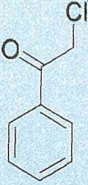
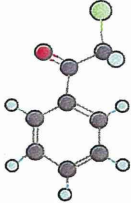

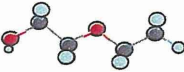
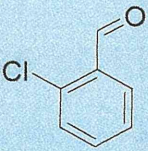
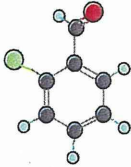
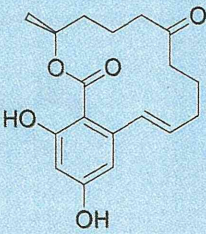
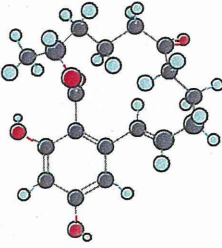
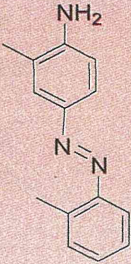
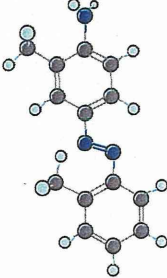
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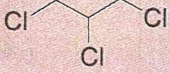
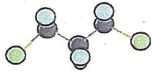
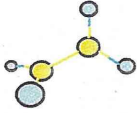
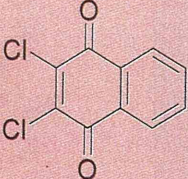
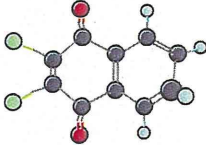
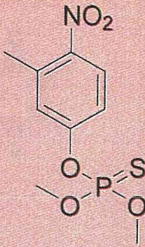
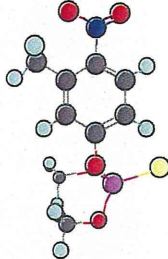
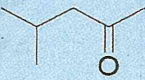
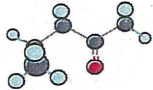
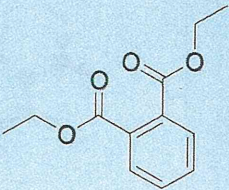
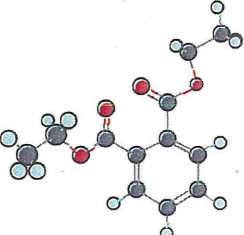
18	 <chem>ClC(Cl)=CCl</chem>	
19	 <chem>OC(=O)c1ccccc1C(=O)O</chem>	
20	 <chem>OC(=O)c1ccccc1C(=O)O</chem>	
21	 <chem>C1CO1</chem>	
22	 <chem>Nc1ccccc1</chem>	
23	 <chem>O=C1OC2=CC=CC=C2C(=O)C1[N+](=O)[O-]</chem>	

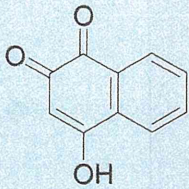
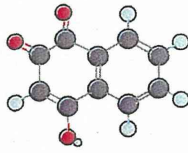
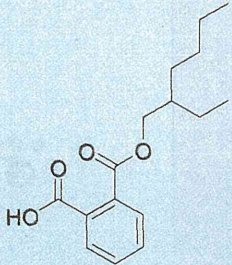
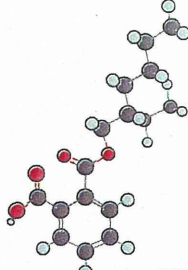

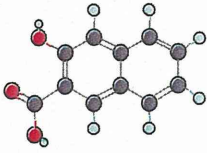

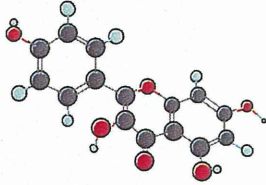
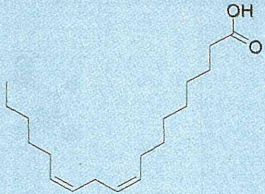
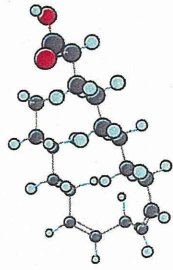
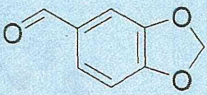
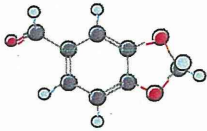
24	 <chem>ClC=CCl</chem>	
25	 <chem>BrC(Br)C</chem>	
26	 <chem>ClC1=CC=C(Cl)C=C1</chem>	
27	 <chem>CCOC(=O)N</chem>	
28	 <chem>N#CC1=CC=CC=C1</chem>	
29	 <chem>CC(=O)NC1=CC=CC=C1</chem>	

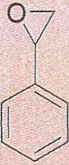
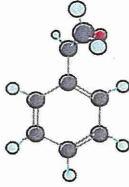
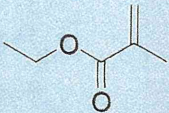
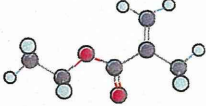
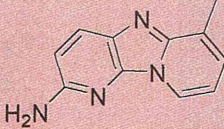
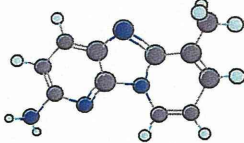

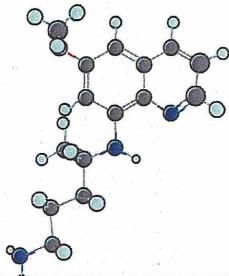
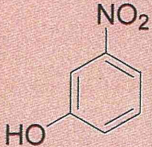
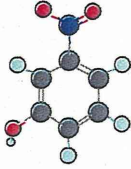
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36	 <p>Chemical structure of 3-nitrobenzoic acid, showing a benzene ring with a nitro group (O_2N) and a carboxylic acid group (COOH) in the meta position.</p>	 <p>Ball-and-stick model of 3-nitrobenzoic acid, showing the spatial arrangement of atoms.</p>
37	 <p>Chemical structure of cyclohexanone oxime, showing a six-membered ring with a double bond to an oxygen atom and a single bond to a nitrogen atom, which is bonded to a hydroxyl group (OH).</p>	 <p>Ball-and-stick model of cyclohexanone oxime, showing the spatial arrangement of atoms.</p>
38	 <p>Chemical structure of dimethyl phthalate, showing a benzene ring with two ester groups (COOCH_3) in the ortho position.</p>	 <p>Ball-and-stick model of dimethyl phthalate, showing the spatial arrangement of atoms.</p>
39	 <p>Chemical structure of acrylamide, showing a vinyl group ($\text{CH}_2=\text{CH}$) attached to an amide group (CONH_2).</p>	 <p>Ball-and-stick model of acrylamide, showing the spatial arrangement of atoms.</p>
40	 <p>Chemical structure of 2-ethyl-1-hexanol, showing a six-carbon chain with a hydroxyl group (HO) at the first carbon and an ethyl group at the second carbon.</p>	 <p>Ball-and-stick model of 2-ethyl-1-hexanol, showing the spatial arrangement of atoms.</p>
41	 <p>Chemical structure of 1-nitro-2,3-dihydro-1H-indene, showing a benzene ring fused to a five-membered ring, with a nitro group (NO_2) at the 1-position.</p>	 <p>Ball-and-stick model of 1-nitro-2,3-dihydro-1H-indene, showing the spatial arrangement of atoms.</p>

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49	$\text{H}_2\text{B}-\text{BH}_2$	
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