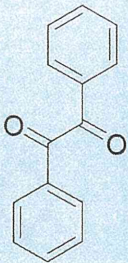
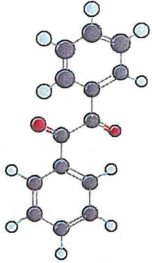
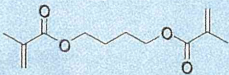
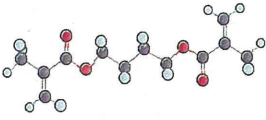
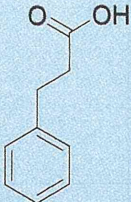
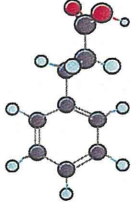
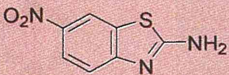

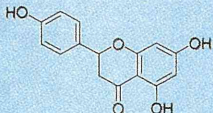
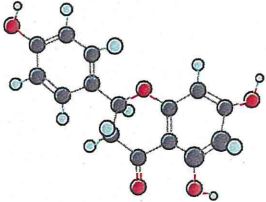
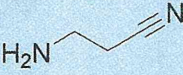
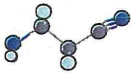


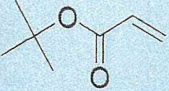
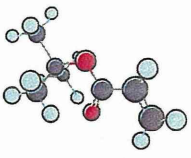

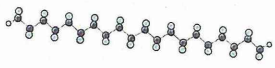
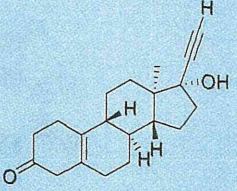
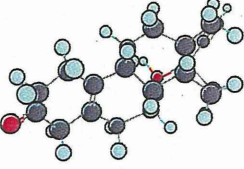
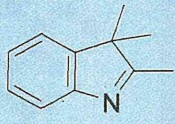
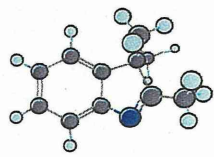
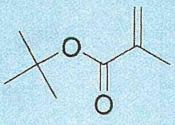
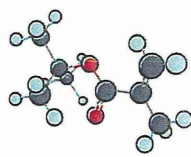
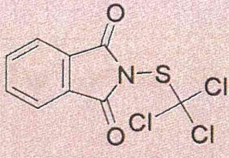
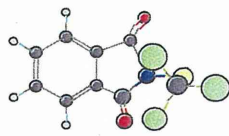
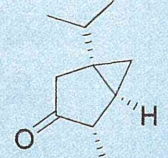
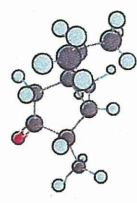

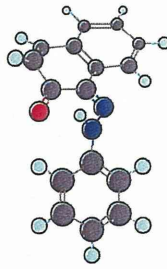
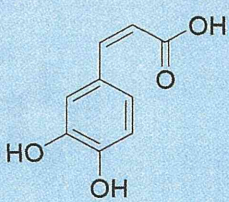
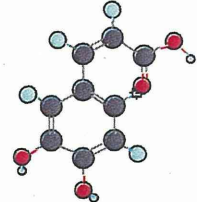
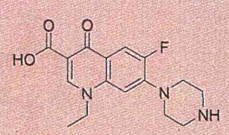
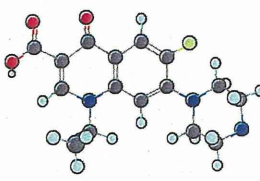
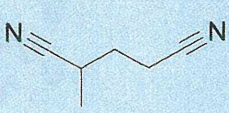
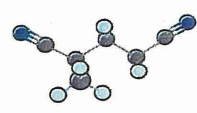
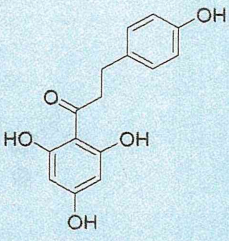
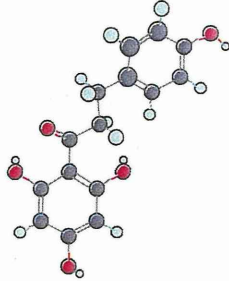
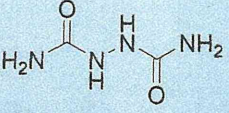
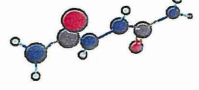
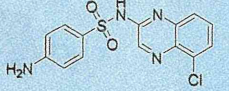
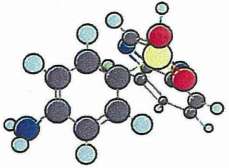

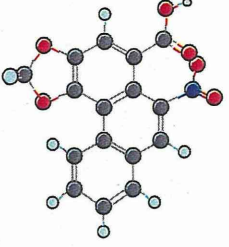
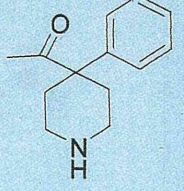
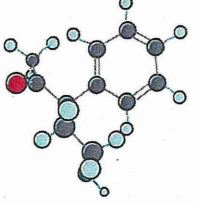

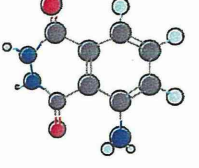


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187	 <chem>CC(C)=COCCOCCCCCOC(=O)C(C)C</chem>	
188	 <chem>OC(=O)Cc1ccccc1</chem>	
189	 <chem>NC1=NC2=CC=C(C=C2S1)[N+](=O)[O-]</chem>	
190	 <chem>Oc1ccc2c(c1)oc(=O)c(O)c2</chem>	
191	 <chem>NCC#N</chem>	

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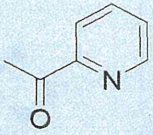
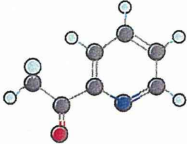
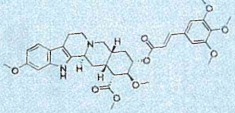
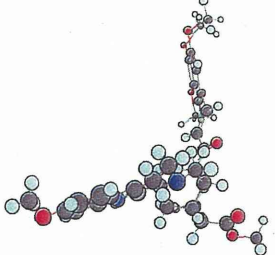
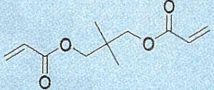
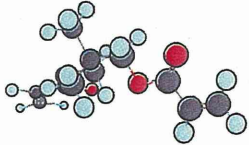
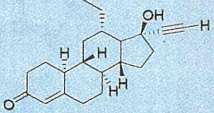
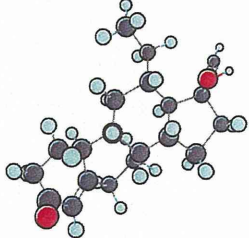
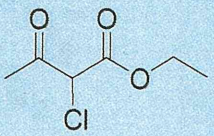
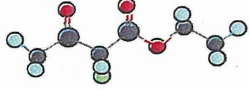
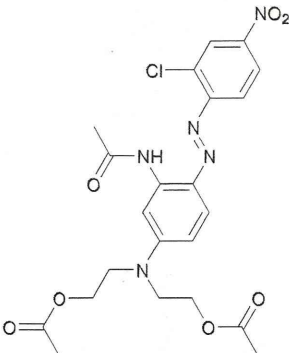
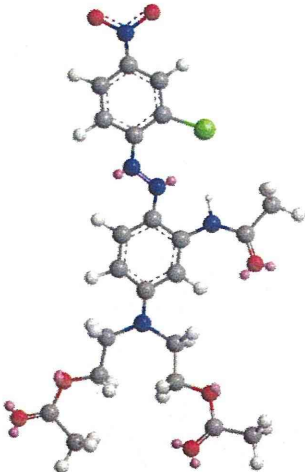
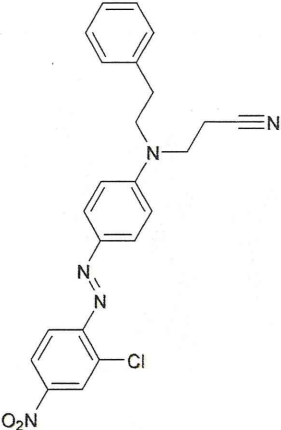
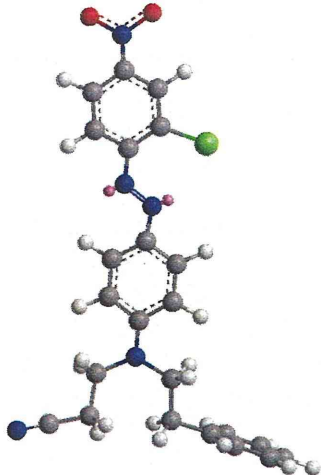
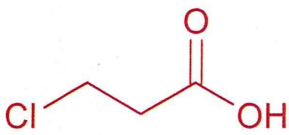
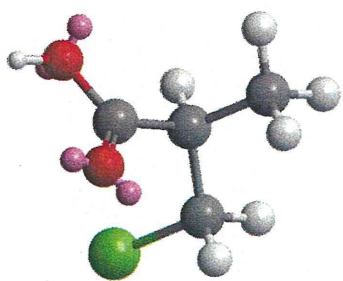
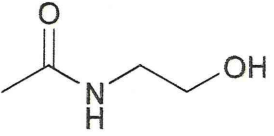
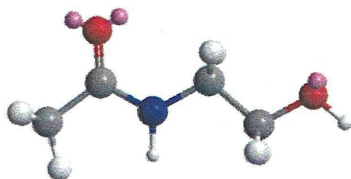
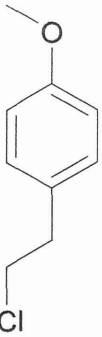
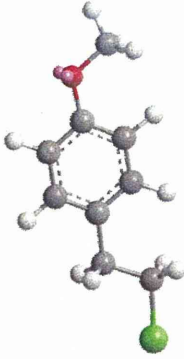
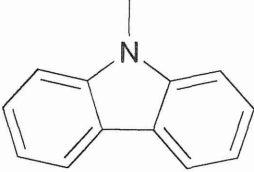
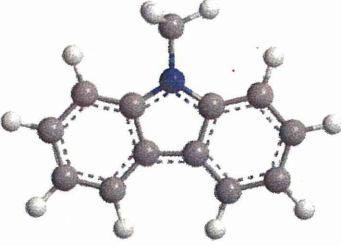
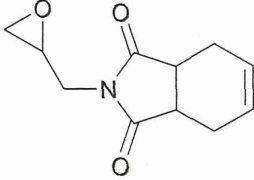
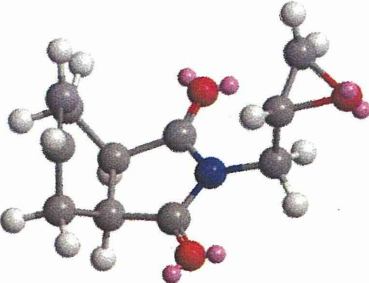
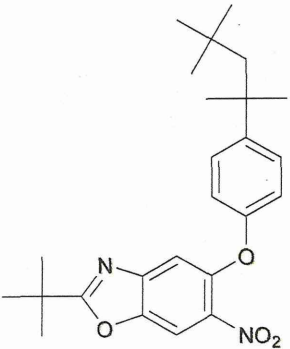
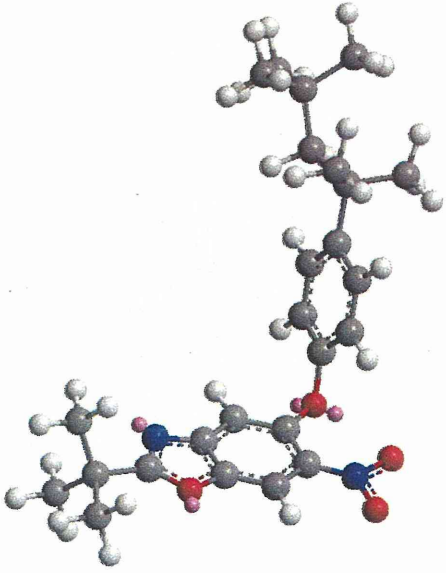
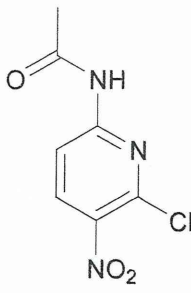
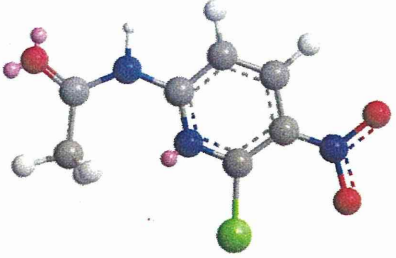
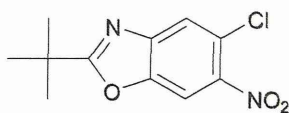
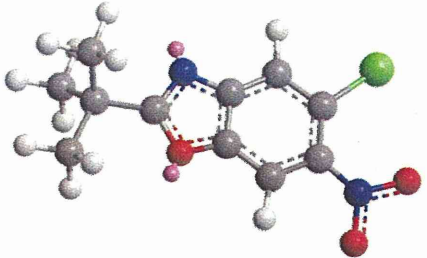
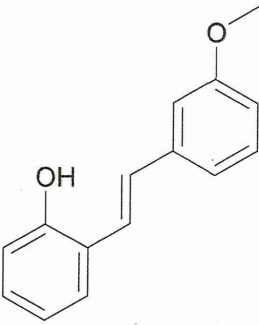
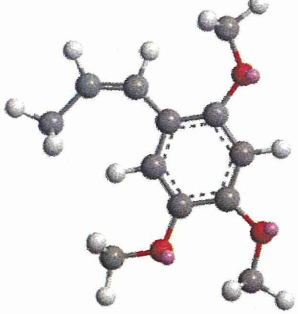
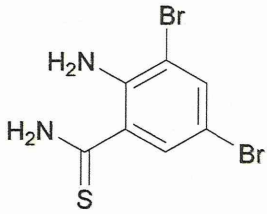
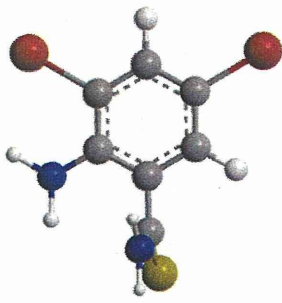
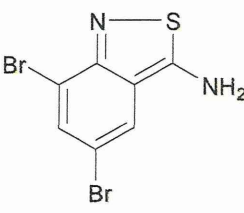
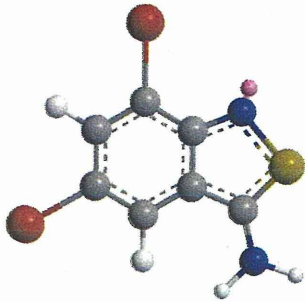
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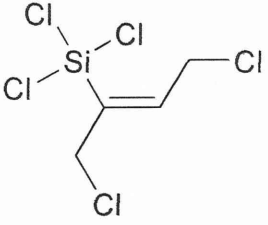
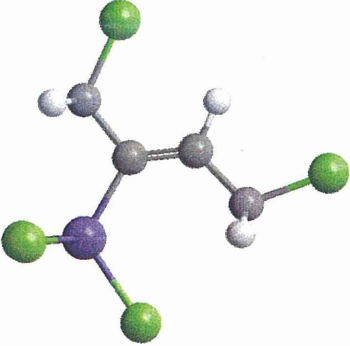
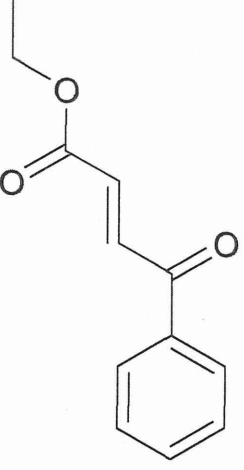
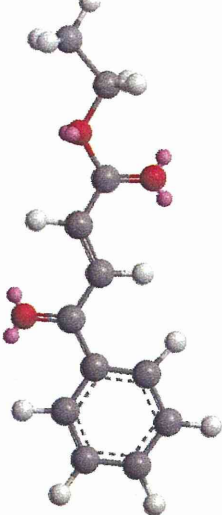
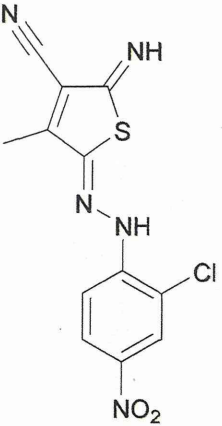
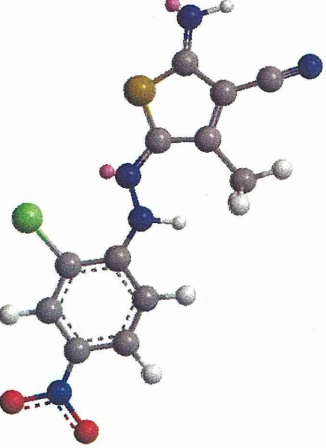
表 14

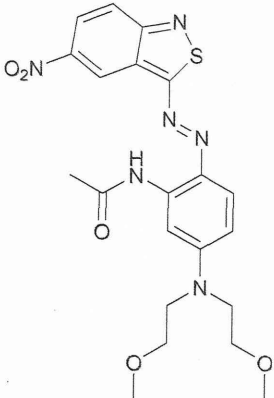
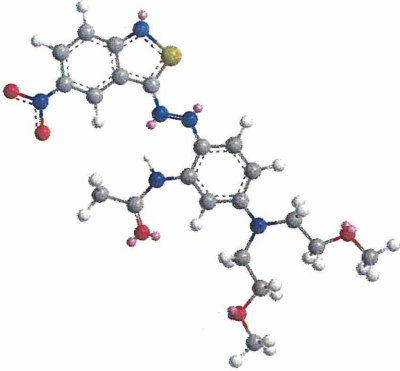
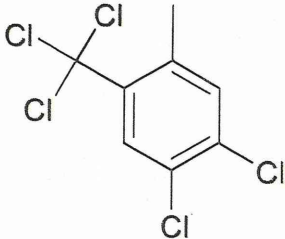
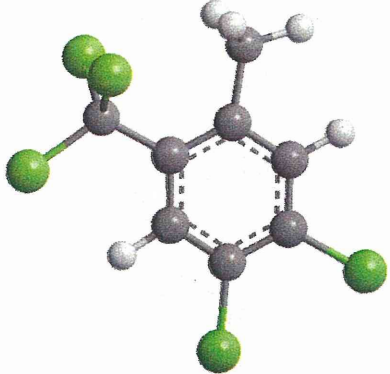
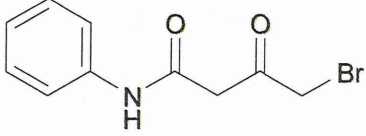
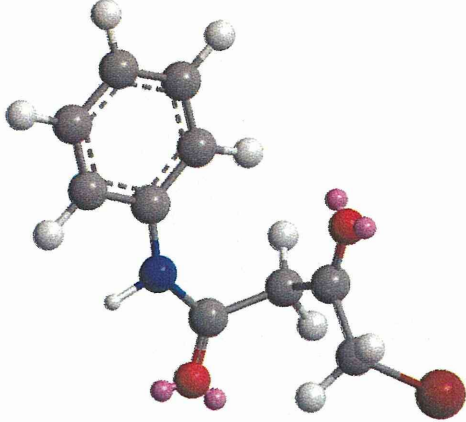
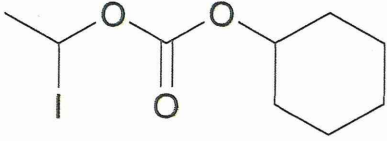
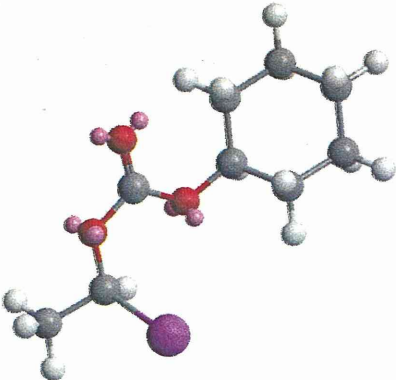
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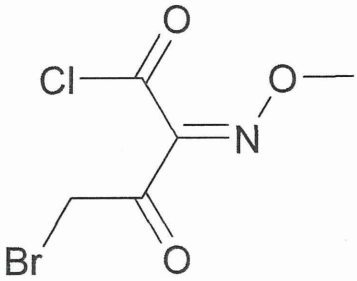
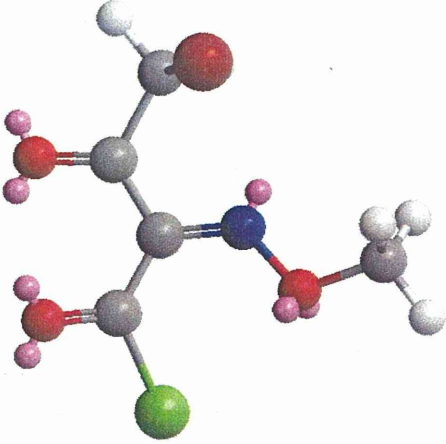
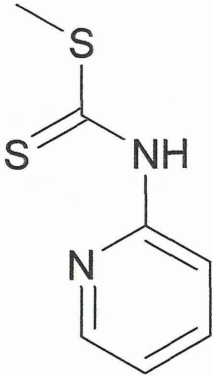
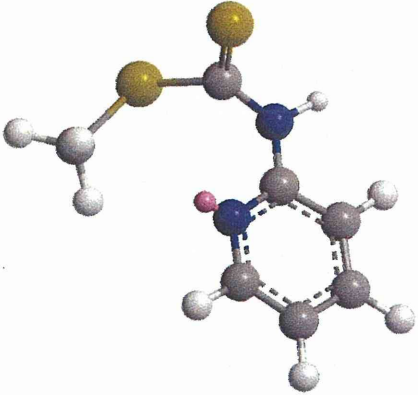
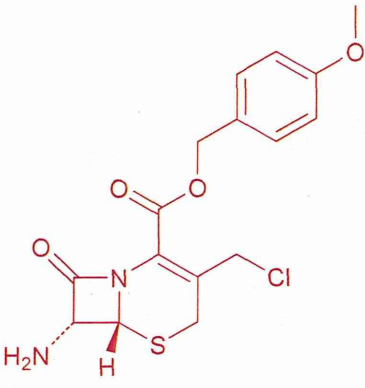
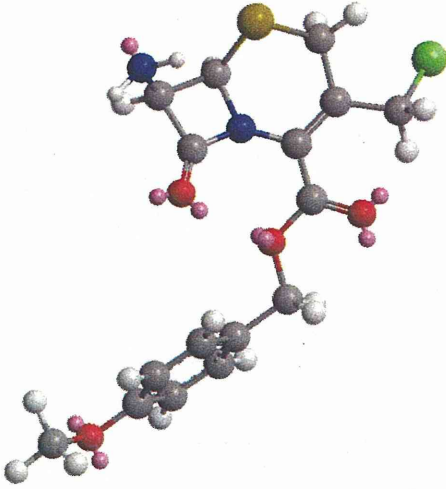
5	 <p>Chemical structure of 4-(chloromethyl)anisole, showing a benzene ring with a methoxy group (-OCH<sub>3</sub>) at the para position and a chloromethyl group (-CH<sub>2</sub>Cl) at the other para position.</p>	 <p>3D ball-and-stick model of 4-(chloromethyl)anisole, showing the spatial arrangement of atoms (Carbon in grey, Oxygen in red, Chlorine in green, Hydrogen in white).</p>
6	 <p>Chemical structure of indole, a bicyclic aromatic heterocycle consisting of a benzene ring fused to a pyrrole ring.</p>	 <p>3D ball-and-stick model of indole, showing the spatial arrangement of atoms (Carbon in grey, Nitrogen in blue, Hydrogen in white).</p>
7	 <p>Chemical structure of 2-(oxiranylmethyl)isoindolin-1-one, featuring an isoindolinone core with an oxirane ring attached to the 2-position.</p>	 <p>3D ball-and-stick model of 2-(oxiranylmethyl)isoindolin-1-one, showing the spatial arrangement of atoms (Carbon in grey, Nitrogen in blue, Oxygen in red, Hydrogen in white).</p>
8	 <p>Chemical structure of a complex substituted benzimidazole derivative. It features a benzimidazole core with a tert-butyl group at the 2-position, a nitro group (-NO<sub>2</sub>) at the 6-position, and a 4-tert-butylphenoxy group at the 7-position.</p>	 <p>3D ball-and-stick model of the complex substituted benzimidazole, showing the spatial arrangement of atoms (Carbon in grey, Nitrogen in blue, Oxygen in red, Hydrogen in white).</p>

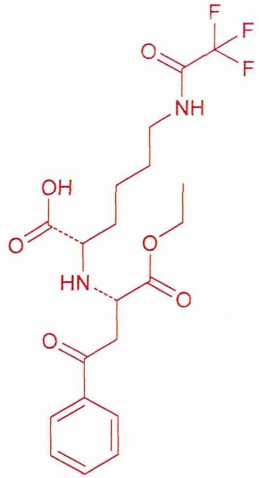
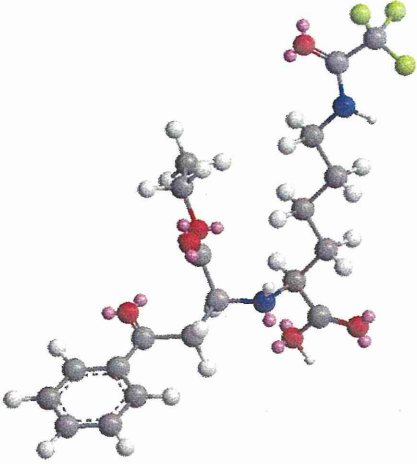
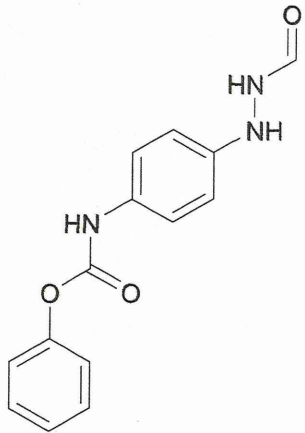
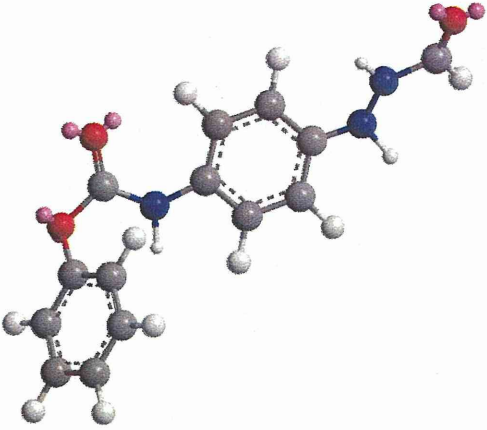
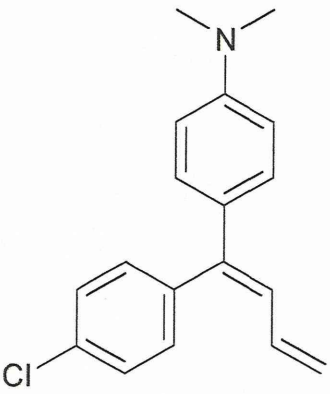
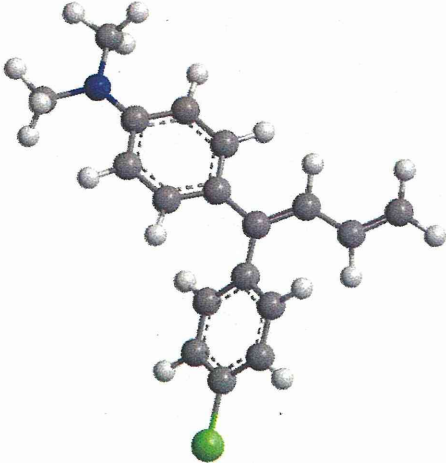
9	 <p>Chemical structure of 2-chloro-4-nitroacetophenone imine. It features a benzene ring with a chlorine atom at the 2-position and a nitro group at the 4-position. An acetophenone imine group is attached to the 1-position of the ring.</p>	 <p>3D ball-and-stick model of 2-chloro-4-nitroacetophenone imine, showing the spatial arrangement of atoms and the orientation of the imine and nitro groups.</p>
10	 <p>Chemical structure of 2-(2-chloro-5-nitrophenyl)isoxazole. It consists of an isoxazole ring system connected to a benzene ring that has a chlorine atom at the 2-position and a nitro group at the 5-position.</p>	 <p>3D ball-and-stick model of 2-(2-chloro-5-nitrophenyl)isoxazole, illustrating the conformation of the isoxazole ring and its attachment to the substituted benzene ring.</p>
11	 <p>Chemical structure of 4-methoxychalcone. It is a chalcone derivative with a hydroxyl group on the phenyl ring of the propenal side chain and a methoxy group on the para position of the other phenyl ring.</p>	 <p>3D ball-and-stick model of 4-methoxychalcone, showing the trans configuration of the propenal side chain and the spatial orientation of the hydroxyl and methoxy groups.</p>
12	 <p>Chemical structure of 2,4-dibromo-5-aminothiobenzamide. It features a benzene ring with bromine atoms at the 2 and 4 positions and an amino group at the 5 position. A thiobenzamide group is attached to the 1 position.</p>	 <p>3D ball-and-stick model of 2,4-dibromo-5-aminothiobenzamide, highlighting the positions of the bromine and amino groups on the benzene ring.</p>
13	 <p>Chemical structure of 2-amino-4,6-dibromo-1,2,4-thiazole. It consists of a 1,2,4-thiazole ring with bromine atoms at the 4 and 6 positions and an amino group at the 2 position.</p>	 <p>3D ball-and-stick model of 2-amino-4,6-dibromo-1,2,4-thiazole, showing the planar nature of the thiazole ring and the orientation of the bromine and amino groups.</p>

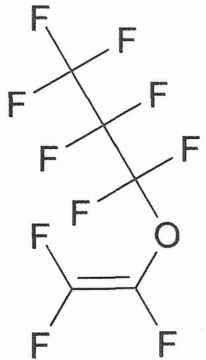
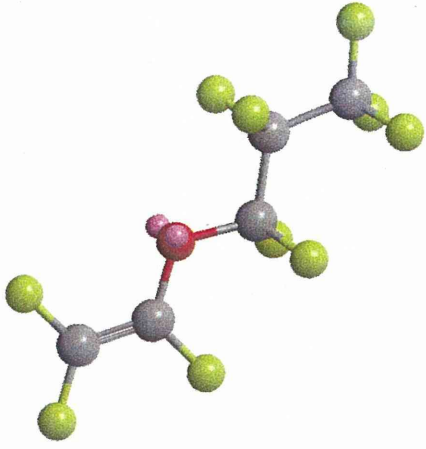
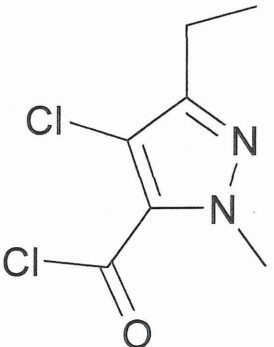
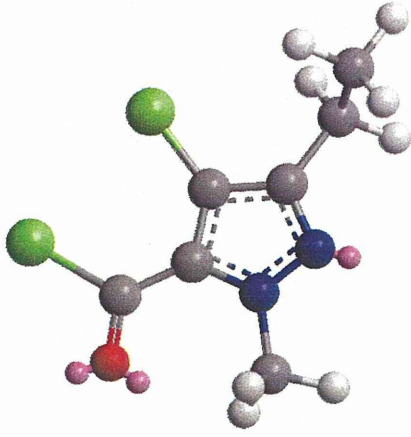
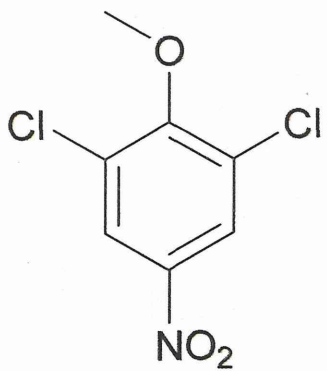
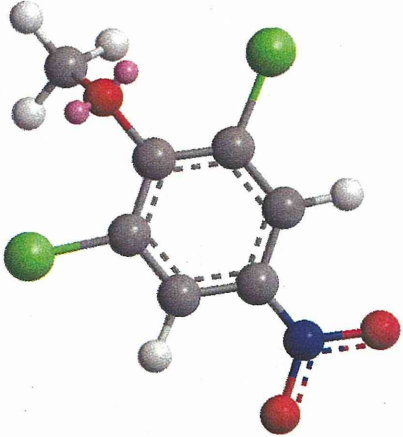
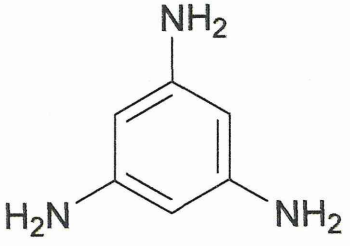
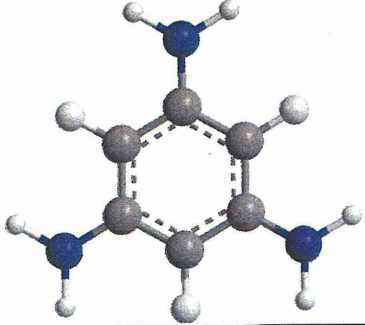


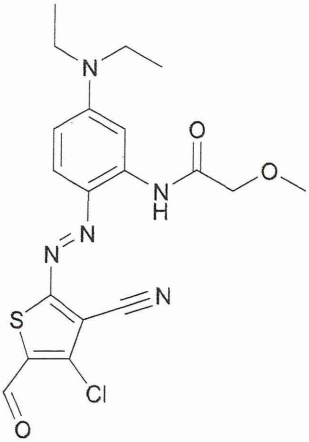
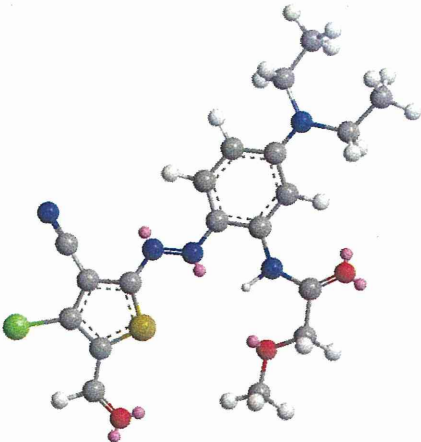
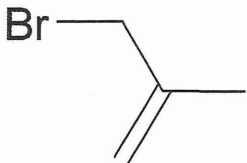
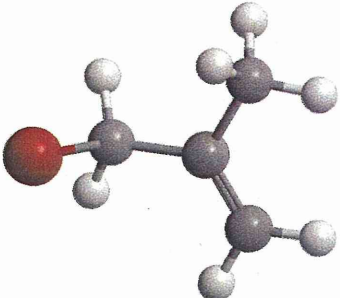
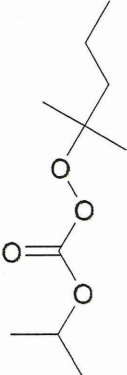
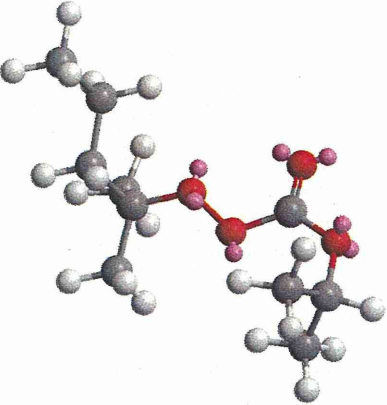
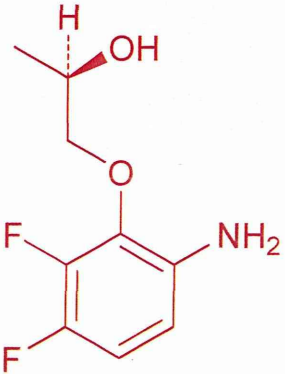
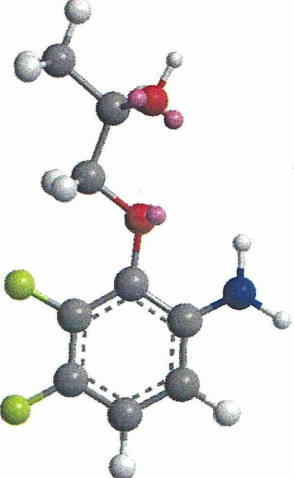
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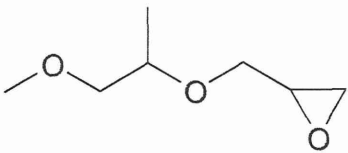
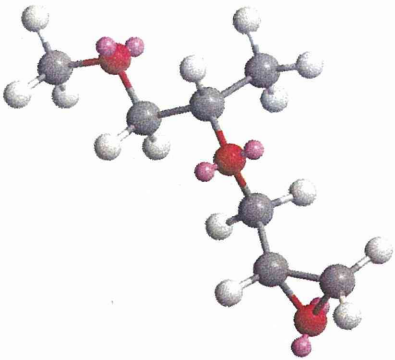
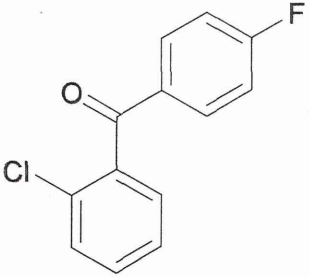
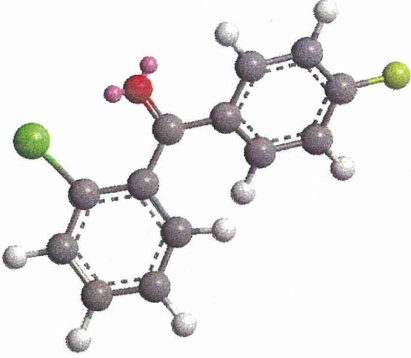
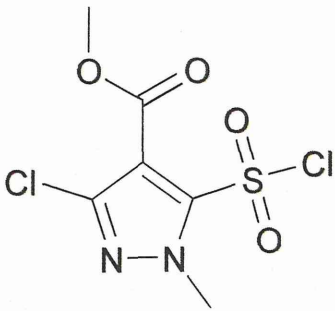
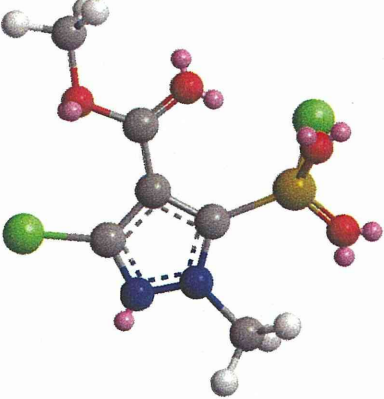
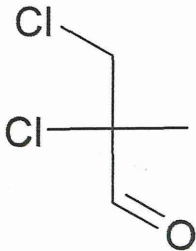
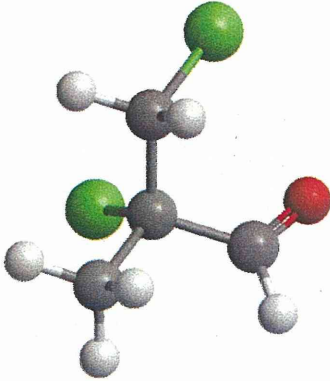
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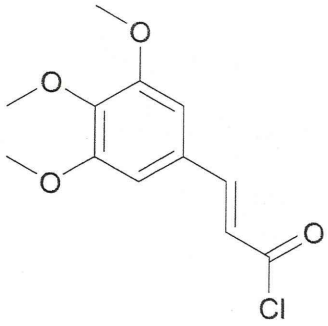
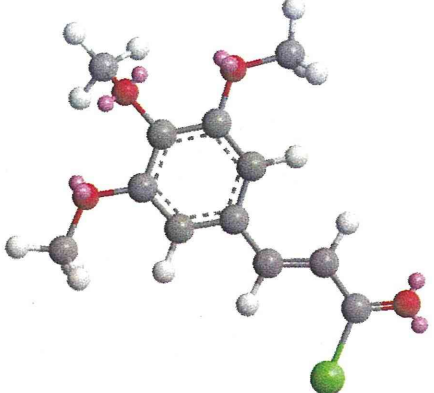
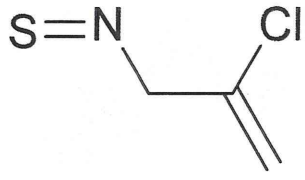
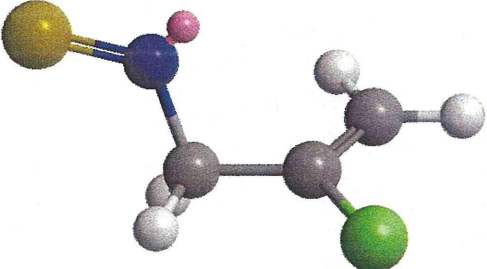
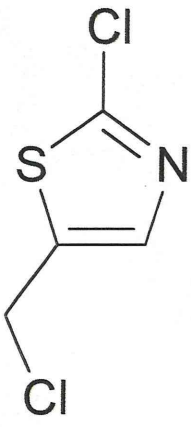
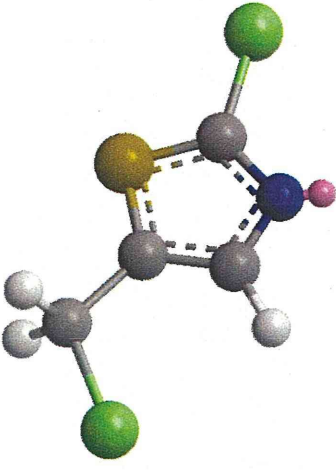
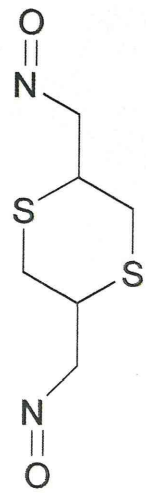
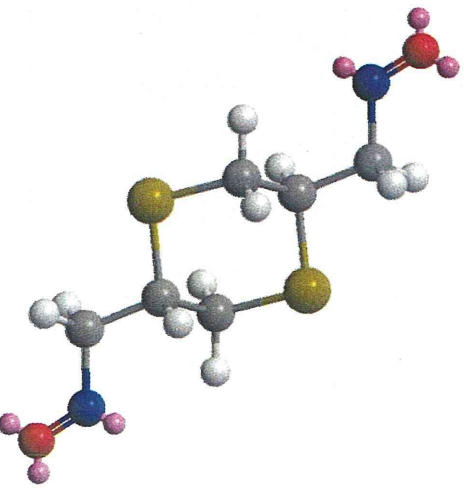
21	 <p>Chemical structure of 2-bromo-3-chloro-N-methoxyacetamide. It features a central carbon atom bonded to a chlorine atom, a bromoethyl group, and an N-methoxyimino group.</p>	 <p>3D ball-and-stick model of 2-bromo-3-chloro-N-methoxyacetamide. The model shows the spatial arrangement of atoms, with carbon in grey, oxygen in red, nitrogen in blue, bromine in green, and hydrogen in white.</p>
22	 <p>Chemical structure of N-(4-methylthio)phenylacetamide. It consists of a phenyl ring attached to an acetamide group, which is further substituted with a methylsulfanyl group.</p>	 <p>3D ball-and-stick model of N-(4-methylthio)phenylacetamide. The model shows the spatial arrangement of atoms, with carbon in grey, oxygen in red, nitrogen in blue, sulfur in yellow, and hydrogen in white.</p>
23	 <p>Chemical structure of a complex heterocyclic molecule. It features a fused bicyclic system with a nitrogen atom, a sulfur atom, and a chlorine atom. The structure is highlighted in red.</p>	 <p>3D ball-and-stick model of the complex heterocyclic molecule. The model shows the spatial arrangement of atoms, with carbon in grey, oxygen in red, nitrogen in blue, sulfur in yellow, chlorine in green, and hydrogen in white.</p>

24	 <p>Chemical structure of a complex molecule featuring a benzene ring, a carboxylic acid group, an amide group, and a trifluoromethyl group.</p>	 <p>3D ball-and-stick model of the molecule shown in the adjacent cell.</p>
25	 <p>Chemical structure of a molecule with a benzene ring, a carbonyl group, and a hydrazine group.</p>	 <p>3D ball-and-stick model of the molecule shown in the adjacent cell.</p>
26	 <p>Chemical structure of a molecule with a benzene ring, a chlorine atom, and a dimethylamino group.</p>	 <p>3D ball-and-stick model of the molecule shown in the adjacent cell.</p>

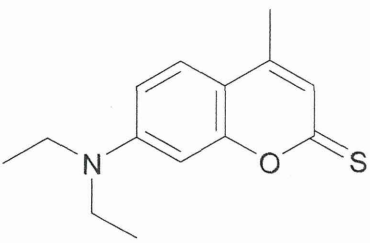
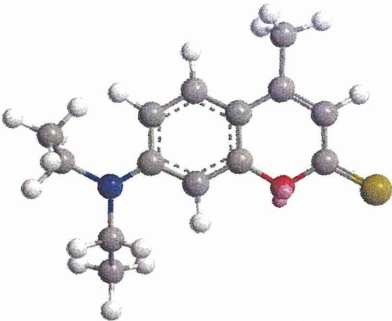
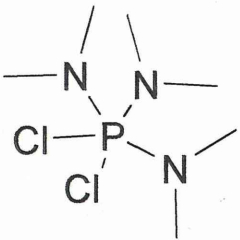
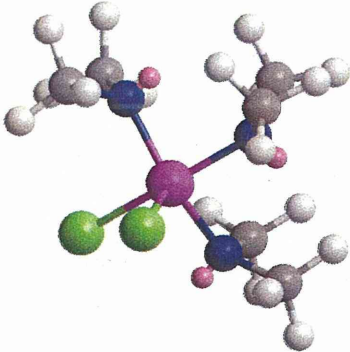
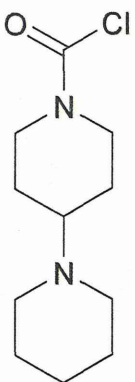
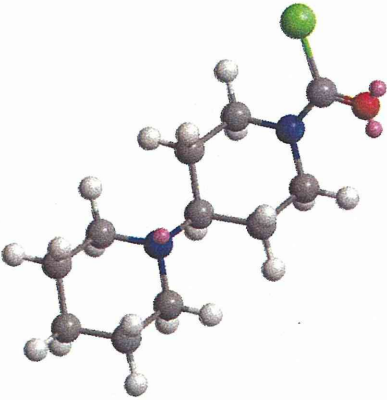
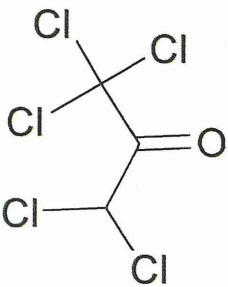
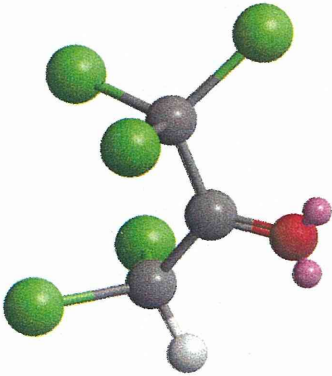
27	 <p>Chemical structure of hexafluorocyclopentadiene, showing a five-membered ring with two double bonds and six fluorine atoms attached to the carbons.</p>	 <p>3D ball-and-stick model of hexafluorocyclopentadiene, showing the spatial arrangement of atoms (carbon in grey, fluorine in yellow, oxygen in red).</p>
28	 <p>Chemical structure of 2-ethyl-4,5-dichloro-1-methylimidazole-3-carboxamide, showing a five-membered imidazole ring with an ethyl group, two chlorine atoms, and a methylamino group, and a carboxamide group attached to the ring.</p>	 <p>3D ball-and-stick model of 2-ethyl-4,5-dichloro-1-methylimidazole-3-carboxamide, showing the spatial arrangement of atoms (carbon in grey, nitrogen in blue, oxygen in red, chlorine in green, hydrogen in white).</p>
29	 <p>Chemical structure of 1-methoxy-2,4-dichloro-5-nitrobenzene, showing a benzene ring with a methoxy group, two chlorine atoms, and a nitro group attached.</p>	 <p>3D ball-and-stick model of 1-methoxy-2,4-dichloro-5-nitrobenzene, showing the spatial arrangement of atoms (carbon in grey, oxygen in red, nitrogen in blue, chlorine in green, hydrogen in white).</p>
30	 <p>Chemical structure of 1,3,5-triaminobenzene, showing a benzene ring with three amino groups attached at the 1, 3, and 5 positions.</p>	 <p>3D ball-and-stick model of 1,3,5-triaminobenzene, showing the spatial arrangement of atoms (carbon in grey, nitrogen in blue, oxygen in red, hydrogen in white).</p>

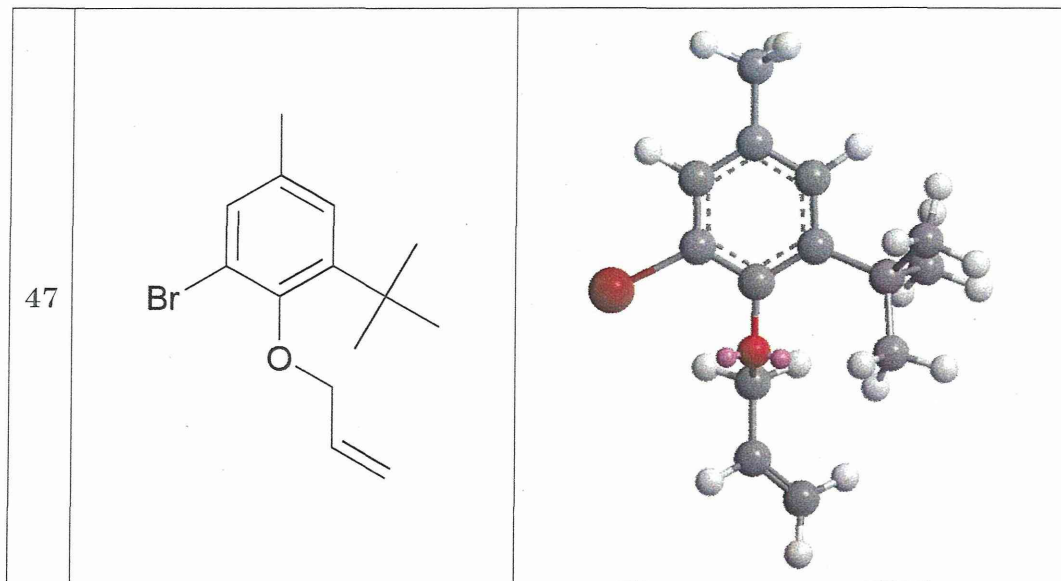
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39	 <p>Chemical structure of 3-(3,4,5-trimethoxyphenyl)acryloyl chloride. It features a benzene ring with three methoxy groups (-OCH<sub>3</sub>) at the 3, 4, and 5 positions, and a propenoate group (-CH=CH-COCl) at the 1 position.</p>	 <p>3D ball-and-stick model of 3-(3,4,5-trimethoxyphenyl)acryloyl chloride. Carbon atoms are grey, oxygen atoms are red, hydrogen atoms are white, and the chlorine atom is green.</p>
40	 <p>Chemical structure of 2-(chloromethyl)acrylonitrile. It consists of a vinyl group (-CH=CH<sub>2</sub>) attached to a methylene group (-CH<sub>2</sub>-) which is further attached to a nitrile group (-C≡N). A chlorine atom is attached to the methylene carbon.</p>	 <p>3D ball-and-stick model of 2-(chloromethyl)acrylonitrile. Carbon atoms are grey, nitrogen is blue, oxygen is red, hydrogen atoms are white, and the chlorine atom is green.</p>
41	 <p>Chemical structure of 2-(chloromethyl)-4-chloro-1,3,4-thiazole. It features a five-membered thiazole ring with a sulfur atom at position 1 and a nitrogen atom at position 3. Chlorine atoms are attached at positions 4 and 5, and a chloromethyl group (-CH<sub>2</sub>Cl) is attached at position 2.</p>	 <p>3D ball-and-stick model of 2-(chloromethyl)-4-chloro-1,3,4-thiazole. Carbon atoms are grey, sulfur is yellow, nitrogen is blue, oxygen is red, hydrogen atoms are white, and chlorine atoms are green.</p>
42	 <p>Chemical structure of 1,3-bis(2-nitroethyl)thiophane. It consists of a six-membered ring with two sulfur atoms at positions 1 and 3, and two ethyl chains at positions 2 and 4. Each ethyl chain has a nitro group (-NO<sub>2</sub>) at the terminal carbon.</p>	 <p>3D ball-and-stick model of 1,3-bis(2-nitroethyl)thiophane. Carbon atoms are grey, sulfur atoms are yellow, nitrogen atoms are blue, oxygen atoms are red, and hydrogen atoms are white.</p>



43	 <p>Chemical structure of 2-(diethylamino)-4-methylthiophene, showing a thiophene ring with a diethylamino group at position 2 and a methyl group at position 4.</p>	 <p>3D ball-and-stick model of 2-(diethylamino)-4-methylthiophene, showing the spatial arrangement of atoms.</p>
44	 <p>Chemical structure of a phosphorus trichloride complex, showing a central phosphorus atom bonded to three chlorine atoms and three nitrogen atoms.</p>	 <p>3D ball-and-stick model of a phosphorus trichloride complex, showing the spatial arrangement of atoms.</p>
45	 <p>Chemical structure of N-(chloroacetyl)pyrrolidine, showing a pyrrolidine ring with a chloroacetyl group attached to the nitrogen atom.</p>	 <p>3D ball-and-stick model of N-(chloroacetyl)pyrrolidine, showing the spatial arrangement of atoms.</p>
46	 <p>Chemical structure of 1,1,1,2,2-pentachloroethane, showing a central carbon atom bonded to three chlorine atoms and another carbon atom bonded to two chlorine atoms and a carbonyl group.</p>	 <p>3D ball-and-stick model of 1,1,1,2,2-pentachloroethane, showing the spatial arrangement of atoms.</p>



予測精度(concordance)

類似度	n	TOP1	TOP3	TOP5	ALL3
0.8	999	0.696	0.686	0.704	0.740
0.85	974	0.698	0.689	0.704	0.742
0.9	811	0.713	0.698	0.711	0.755
0.91	752	0.714	0.702	0.713	0.754
0.92	684	0.703	0.699	0.709	0.746
0.93	596	0.698	0.698	0.703	0.740
0.94	503	0.708	0.714	0.720	0.755
0.95	388	0.719	0.714	0.719	0.754
0.96	275	0.738	0.735	0.742	0.778
0.97	147	0.776	0.782	0.762	0.810
0.98	52	0.827	0.808	0.788	0.826
0.99	25	1.000	0.920	0.880	1.000
1	22	1.000	0.909	0.864	1.000

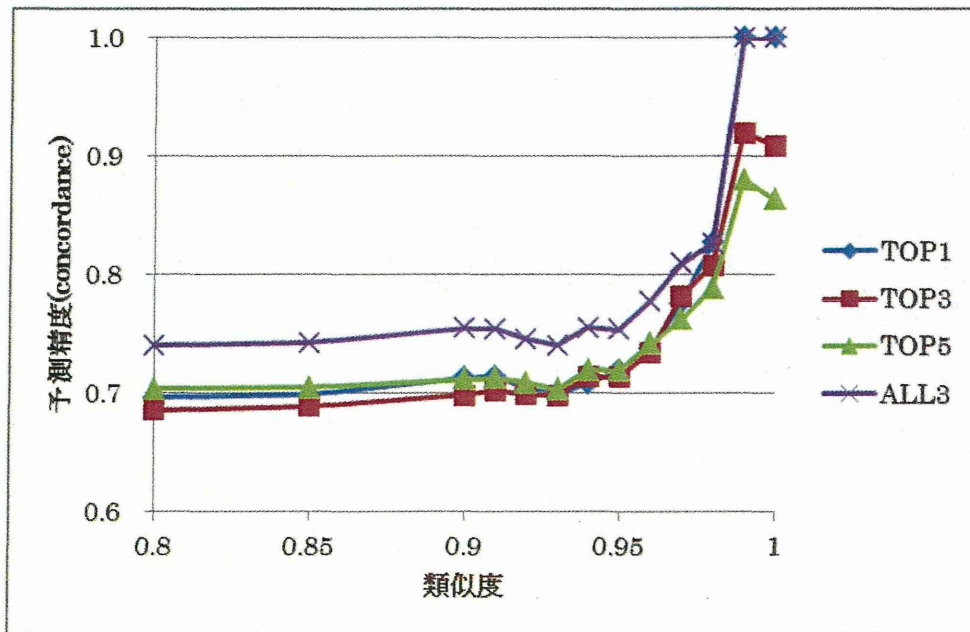


図 1

特異度(specificity)

類似度	n	TOP1	TOP3	TOP5	ALL3
0.8	999	0.725	0.722	0.749	0.781
0.85	974	0.728	0.726	0.751	0.784
0.9	811	0.748	0.737	0.761	0.801
0.91	752	0.747	0.735	0.756	0.795
0.92	684	0.737	0.733	0.753	0.788
0.93	596	0.733	0.735	0.752	0.787
0.94	503	0.734	0.745	0.766	0.794
0.95	388	0.754	0.754	0.772	0.798
0.96	275	0.758	0.767	0.779	0.804
0.97	147	0.795	0.795	0.787	0.827
0.98	52	0.826	0.804	0.804	0.829
0.99	25	1.000	0.909	0.909	1.000
1	22	1.000	0.895	0.895	1.000

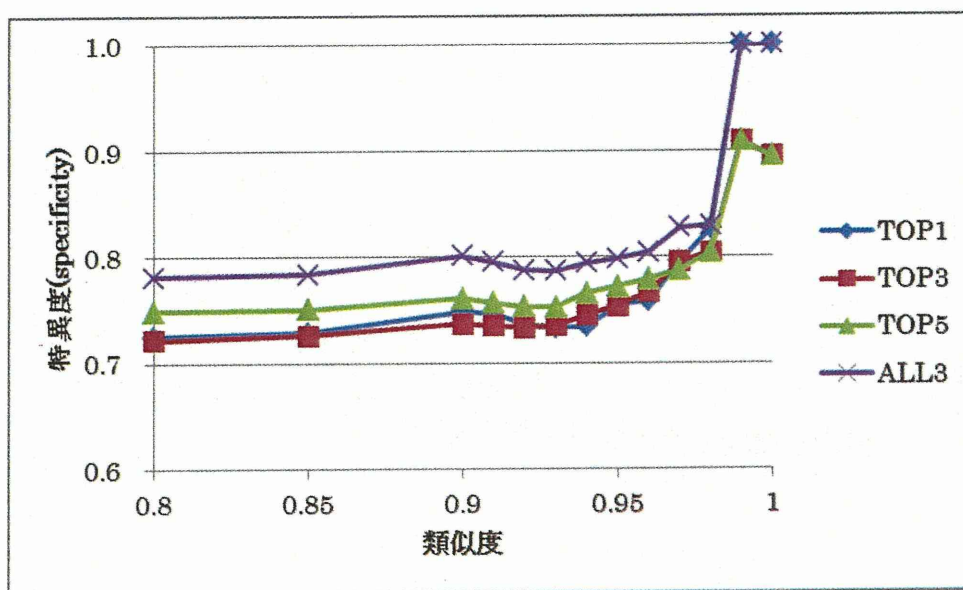


图 2