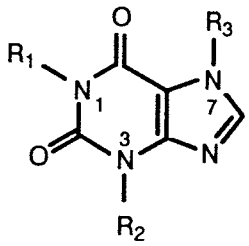
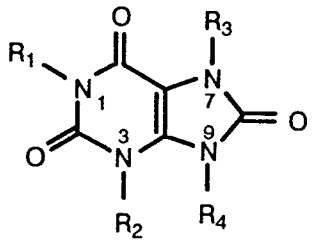
Appendix 1
Chemical formulae of selected components of coffee

1. Nonvolatile compounds

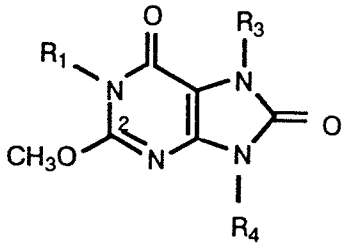
(*a*) *Caffeine and other purines*



$R_1 = R_2 = R_3 = CH_3$: Caffeine, 1,3,7-trimethylxanthine
$R_1 = H$, $R_2 = R_3 = CH_3$: Theobromine, 3,7-dimethylxanthine
$R_1 = R_2 = CH_3$, $R_3 = H$: Theophylline, 1,3-dimethylxanthine
$R_1 = R_3 = CH_3$, $R_2 = H$: Paraxanthine, 1,7-dimethylxanthine

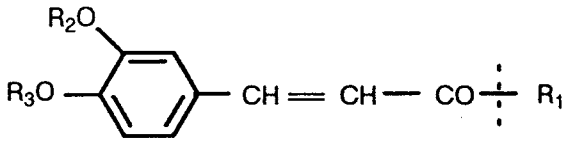


$R_1 = R_2 = R_3 = R_4 = CH_3$: Theacrine, 1,3,7,9-tetramethyluric acid

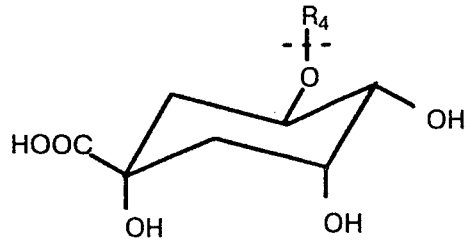


$R_1 = R_4 = CH_3$, $R_3 = H$: Liberine, 0(2), 1,9-trimethyluric acid

(*b*) *Chlorogenic acid and related substances*



A (R_2 = R_3 = H): Caffeoyl

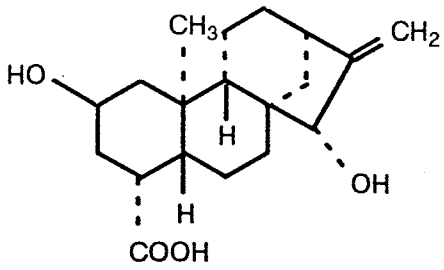


B: Quinyl

R_1 = B, R_2 = R_3 = H, R_4 = A:	Chlorogenic acid
R_1 = OH, R_2 = R_3 = H:	Caffeic acid
R_1 = OH, R_2 = H, R_3 = CH_3:	Ferulic acid
R_1 = OH, R_2 = CH_3, R_3 = H:	Isoferulic acid
R_4 = H:	Quinic acid

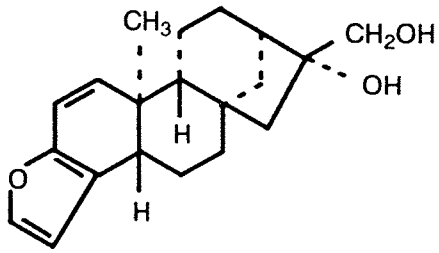
A chlorogenic acid (taken as 5-caffeoylquinic acid) and component acids

(*c*) *Glycosides*

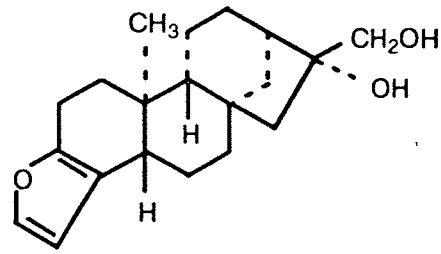


Atractyligenin

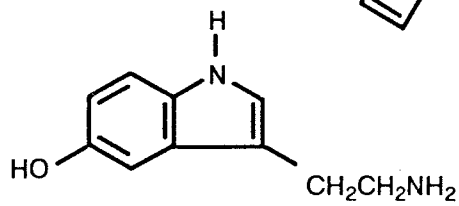
(*d*) *Lipids*



Kahweol

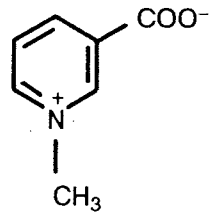


Cafestol

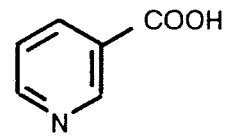


5–Hydroxytryptamine

(*e*) *Trigonelline and nicotinic acid*

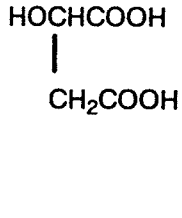


Trigonelline

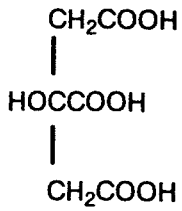


Nicotinic acid

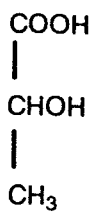
(f) *Acids*



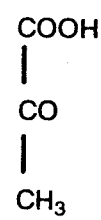
Malic acid



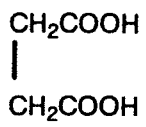
Citric acid



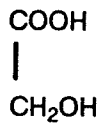
Lactic acid



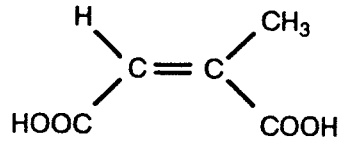
Pyruvic acid



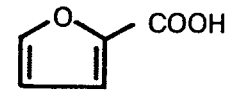
Succinic acid



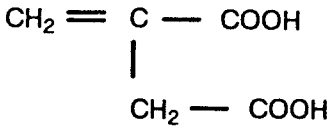
Glycolic acid



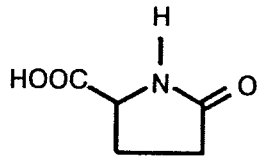
Citraconic acid



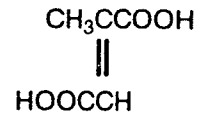
2-Furoic acid



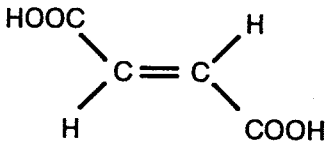
Itaconic acid



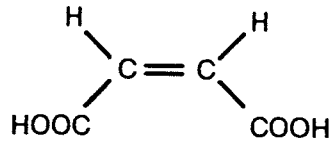
Pyrrolidone carboxylic acid



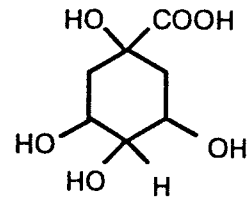
Mesaconic acid



Fumaric acid



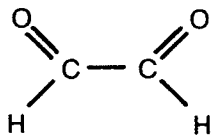
Maleic acid



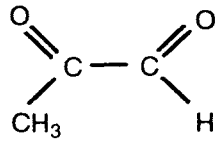
Quinic acid

2. Volatile compounds

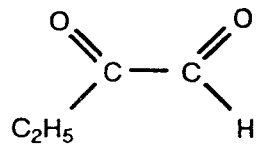
(*a*) *Carbonyl compounds*



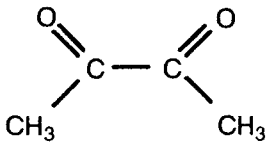
Glyoxal



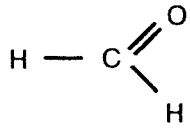
Methylglyoxal



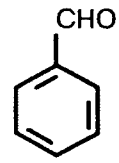
Ethylglyoxal



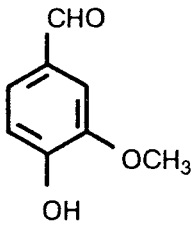
Diacetyl



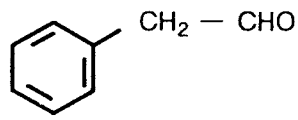
Formaldehyde



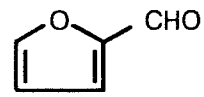
Benzaldehyde



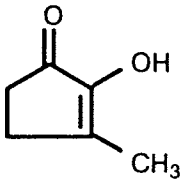
Vanillin



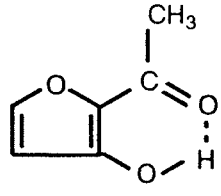
2-Phenylacetaldehyde



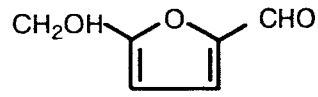
Furfural



Cyclotene

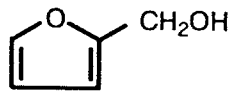


Isomaltol



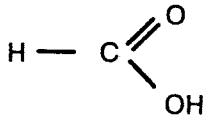
5-(Hydroxymethyl)-2-furfural

(*b*) *Alcohols*



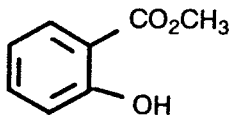
Furfuryl alcohol

(*c*) *Acids*



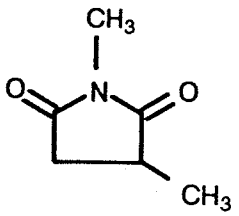
Formic acid

(*d*) *Esters, ethers and lactones*

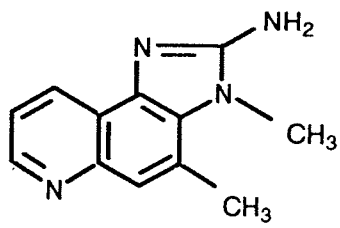


Methyl salicylate

(*e*) *Nitrogen compounds*

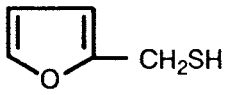


N-α-Dimethylsuccinimide

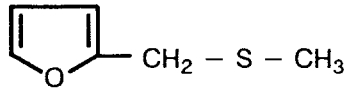


MeIQ

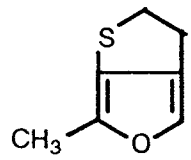
(*f*) *Furan–based compounds*



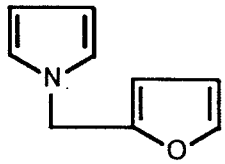
Furfurylthiol



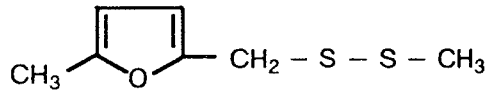
Furfuryl methyl sulfide



Kahweofuran

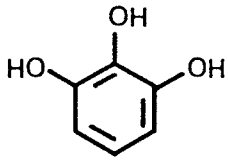


N-Furfurylpyrrole

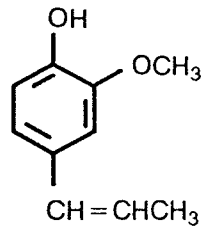


5-Methylfurfuryl methyl disulfide

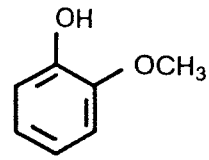
(*g*) *Phenols*



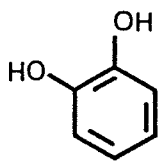
Pyrogallol



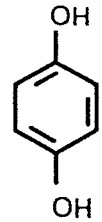
Isoeugenol



Guaiacol

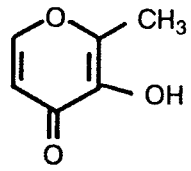


Pyrocatechol



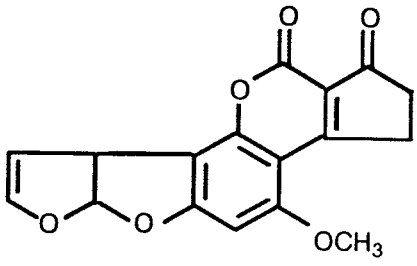
Hydroquinone

(*h*) Pyrones

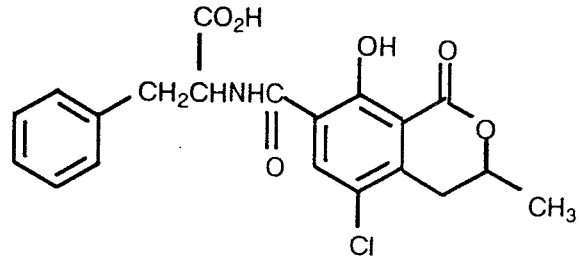


Maltol

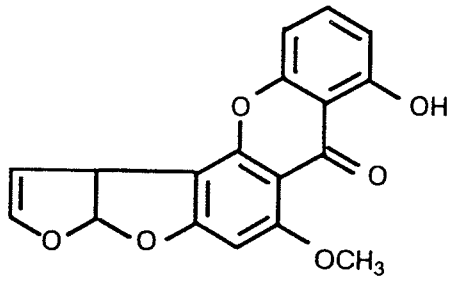
(*i*) *Contaminants*



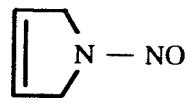
Aflatoxin B_1



Ochratoxin A



Sterigmatocystin



N-Nitrosopyrrolidine