

Appendix 1
**Occurrence of flavour compounds and some other
compounds in alcoholic beverages**

Appendix 1. Occurrence of flavour compounds and some other compounds in alcoholic beverages^a

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits

FLAVOUR COMPOUNDS				
Aliphatic monohydric alcohols				
Methanol	CH ₄ O			+
Allyl alcohol (2-Propen-1-ol)	C ₃ H ₆ O			+
1-Propanol	C ₃ H ₈ O	+	+	+
Isopropyl alcohol (IARC, 1977b, 1987a)	C ₃ H ₈ O	+	+	+
2-Methyl-1-propanol	C ₄ H ₁₀ O	+	+	+
n-Butyl alcohol (1-Butanol)	C ₄ H ₁₀ O	+	+	+
sec-Butyl alcohol (2-Butanol)	C ₄ H ₁₀ O	+	+	+
tert-Butyl alcohol (2-Methyl-2-propanol)	C ₄ H ₁₀ O		+	
Methylbutenol	C ₅ H ₁₀ O			+
2-Methyl-3-buten-2-ol	C ₅ H ₁₀ O	+		
2-Methyl-1-butanol	C ₅ H ₁₂ O	+	+	+
Pentyl alcohol (1-Pentanol)	C ₅ H ₁₂ O	+	+	+
3-Methyl-1-butanol	C ₅ H ₁₂ O	+	+	+
tert-Pentyl alcohol (2-Methyl-2-butanol)	C ₅ H ₁₂ O	+	+	+
2-Pentanol	C ₅ H ₁₂ O	+	+	+
3-Pentanol	C ₅ H ₁₂ O		+	+
2,4-Hexadien-1-ol, trans,trans-	C ₆ H ₁₀ O		+	
2-Hexen-1-ol	C ₆ H ₁₂ O	+		
2-Hexen-1-ol, cis-				+
2-Hexen-1-ol, trans-		+	+	+
3-Hexenol	C ₆ H ₁₂ O	+		
3-Hexenol, cis-		+	+	+
3-Hexenol, trans-			+	+
3-Methyl-1-pentanol	C ₆ H ₁₄ O		+	+
4-Methyl-1-pentanol	C ₆ H ₁₄ O		+	+
N-Hexyl alcohol (1-Hexanol)	C ₆ H ₁₄ O	+	+	+
4-Methyl-2-pentanol	C ₆ H ₁₄ O			+
2-Hexanol	C ₆ H ₁₄ O	+	+	+
3-Hexanol	C ₆ H ₁₄ O			+
2-Hepten-1-ol, trans-	C ₇ H ₁₄ O			+
1-Hepten-3-ol	C ₇ H ₁₄ O	+		+
5-Methyl-1-hexanol	C ₇ H ₁₆ O			+
n-Heptyl alcohol (1-Heptanol)	C ₇ H ₁₆ O	+	+	+
2-Heptanol	C ₇ H ₁₆ O	+	+	+
3-Heptanol	C ₇ H ₁₆ O			+

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
4-Heptanol	C ₇ H ₁₆ O			+
2-Octen-1-ol, <i>trans</i> -	C ₈ H ₁₆ O			+
1-Octen-3-ol	C ₈ H ₁₆ O	+	+	+
6-Methyl-1-heptanol	C ₈ H ₁₈ O		+	
2-Ethyl-1-hexanol	C ₈ H ₁₈ O	+	+	+
<i>n</i> -Octyl alcohol (1-Octanol)	C ₈ H ₁₈ O	+	+	+
2-Octanol	C ₈ H ₁₈ O	+	+	+
3-Octanol	C ₈ H ₁₈ O		+	+
2-Nonen-1-ol, <i>trans</i> -	C ₉ H ₁₈ O			+
2,6-Dimethyl-4-heptanol	C ₉ H ₂₀ O			+
<i>n</i> -Nonyl alcohol (1-Nonanol)	C ₉ H ₂₀ O	+	+	+
2-Nonanol	C ₉ H ₂₀ O	+	+	+
9-Decen-1-ol	C ₁₀ H ₂₀ O			+
<i>n</i> -Decyl alcohol (1-Decanol)	C ₁₀ H ₂₂ O	+	+	+
2-Decanol	C ₁₀ H ₂₂ O	+	+	+
3-Decanol	C ₁₀ H ₂₂ O			+
6-Undecen-2-ol	C ₁₁ H ₂₂ O			
6-Undecen-2-ol, <i>cis</i> -				+
6-Undecen-2-ol, <i>trans</i> -				+
<i>n</i> -Undecyl alcohol (1-Undecanol)	C ₁₁ H ₂₄ O		+	+
2-Undecanol	C ₁₁ H ₂₄ O		+	+
<i>n</i> -Dodecyl alcohol (1-Dodecanol)	C ₁₂ H ₂₆ O	+	+	+
2-Dodecanol	C ₁₂ H ₂₆ O	+	+	
1-Tetradecanol	C ₁₄ H ₃₀ O		+	+
1-Pentadecanol	C ₁₅ H ₃₂ O		+	
1-Hexadecanol	C ₁₆ H ₃₄ O			+
Octadecanol	C ₁₈ H ₃₈ O			+
<i>Aliphatic aldehydes</i>				
Formaldehyde (IARC, 1982a, 1987a)	CH ₂ O	+	+	+
Glyoxal	C ₂ H ₂ O ₂	+		+
Acetaldehyde (IARC, 1985, 1987a)	C ₂ H ₄ O	+	+	+
Glycolic aldehyde	C ₂ H ₄ O ₂		+	
Acrolein (IARC, 1985, 1987a)	C ₃ H ₄ O	+		+
Pyrvaldehyde	C ₃ H ₄ O ₂	+		+
Malonaldehyde (IARC, 1985, 1987a)	C ₃ H ₄ O ₂	+		
Propionaldehyde	C ₃ H ₆ O	+	+	+
Glyceraldehyde	C ₃ H ₆ O ₃	+		
2-Methyl-2-propenal	C ₄ H ₆ O			+
Crotonaldehyde	C ₄ H ₆ O	+		+
Isobutyraldehyde	C ₄ H ₈ O	+	+	+
Butyraldehyde	C ₄ H ₈ O	+	+	+
3-Hydroxybutyraldehyde	C ₄ H ₈ O ₂	+		
Pentadienal	C ₅ H ₆ O	+		
2-Methyl-2-butenal, <i>cis</i> -	C ₅ H ₈ O			+

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
3-Methyl-2-butenal	C ₅ H ₈ O			+
2-Pentenal	C ₅ H ₈ O			+
2-Pentenal, <i>trans</i> -				+
Glutaraldehyde	C ₅ H ₈ O ₂	+		
2-Methylbutyraldehyde	C ₅ H ₁₀ O	+	+	+
Isovaleraldehyde	C ₅ H ₁₀ O	+	+	+
Valeraldehyde	C ₅ H ₁₀ O	+	+	+
2-Ethoxypropionaldehyde	C ₅ H ₁₀ O ₂			+
3-Ethoxypropionaldehyde	C ₅ H ₁₀ O ₂			+
5-Hydroxyvaleraldehyde	C ₅ H ₁₀ O ₂	+		
Hexadienal	C ₆ H ₈ O	+		
2,4-Hexadienal	C ₆ H ₈ O	+		
2,4-Hexadienal, <i>trans,trans</i> -		+		
2-Methyl-2-pentenal, <i>trans</i> -	C ₆ H ₁₀ O			+
2-Hexenal	C ₆ H ₁₀ O	+	+	
2-Hexenal, <i>trans</i> -		+		+
3-Methylvaleraldehyde	C ₆ H ₁₂ O	+		
Hexanal	C ₆ H ₁₂ O	+	+	+
1-Cyclohexene-1-carboxaldehyde	C ₇ H ₁₀ O			+
2-Heptenal, <i>trans</i> -	C ₇ H ₁₂ O	+		+
4-Heptenal	C ₇ H ₁₂ O	+		
Octadienal	C ₈ H ₁₂ O	+		
Octadienal, <i>trans,trans</i> -		+		
2-Octenal, <i>trans</i> -	C ₈ H ₁₄ O			+
Octanal	C ₈ H ₁₆ O	+	+	+
2,4-Nonadienal, <i>trans,trans</i> -	C ₉ H ₁₄ O	+		+
2,6-Nonadienal, <i>trans,cis</i> -	C ₉ H ₁₄ O	+		
2-Nonenal	C ₉ H ₁₆ O	+		
2-Nonenal, <i>trans</i> -		+		+
Nonanal	C ₉ H ₁₈ O	+	+	+
2,2,3-Trimethyl-3-cyclopentenyl-1-acetaldehyde	C ₁₀ H ₁₆ O			+
Decadienal	C ₁₀ H ₁₆ O	+		
2,4-Decadienal, <i>trans,trans</i> -	C ₁₀ H ₁₆ O			+
2-Decenal, <i>trans</i> -	C ₁₀ H ₁₈ O			+
Decanal	C ₁₀ H ₂₀ O	+	+	+
Undecanal	C ₁₁ H ₂₂ O		+	+
Lauraldehyde	C ₁₂ H ₂₄ O	+	+	+
Myristaldehyde	C ₁₄ H ₂₈ O		+	
<i>Aliphatic ketones</i>				
Acetone	C ₃ H ₆ O	+	+	+
1-Hydroxy-2-propanone	C ₃ H ₆ O ₂	+	+	+
Dihydroxyacetone	C ₃ H ₆ O ₃		+	
2,3-Butanedione (Diacetyl)	C ₄ H ₆ O ₂	+	+	+
2-Butanone	C ₄ H ₈ O	+	+	+

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
3-Hydroxy-2-butanone	C ₄ H ₈ O ₂	+	+	+
1,2-Cyclopentanedione	C ₅ H ₆ O ₂			+
Cyclopentanone	C ₅ H ₈ O			+
3-Penten-2-one	C ₅ H ₈ O			+
3-Penten-2-one, <i>trans</i> -				+
2,3-Pentanedione	C ₅ H ₈ O ₂	+	+	+
3-Methyl-2-butanone	C ₅ H ₁₀ O	+		+
2-Pentanone	C ₅ H ₁₀ O	+	+	+
3-Pentanone	C ₅ H ₁₀ O	+	+	
3-Hydroxy-2-pentanone	C ₅ H ₁₀ O ₂	+		
2-Hydroxy-3-methyl-2-cyclopenten-1-one	C ₆ H ₈ O ₂	+		
5-Methyl-1,2-cyclopentanedione	C ₆ H ₈ O ₂			+
2-Methyl-1,3-cyclopentanedione	C ₆ H ₈ O ₂	+		
4-Methyl-3-penten-2-one	C ₆ H ₁₀ O		+	+
5-Hexen-2-one	C ₆ H ₁₀ O	+		
2-Methylcyclopentanone	C ₆ H ₁₀ O			+
2,3-Hexanedione	C ₆ H ₁₀ O ₂	+		
2,5-Hexanedione	C ₆ H ₁₀ O ₂	+		
3-Methyl-2-pentanone	C ₆ H ₁₂ O	+		
4-Methyl-2-pentanone	C ₆ H ₁₂ O	+		+
2-Hexanone	C ₆ H ₁₂ O	+	+	+
3-Hexanone	C ₆ H ₁₂ O	+	+	+
4-Ethoxy-2-butanone	C ₆ H ₁₂ O ₂			+
4-Hydroxy-4-methyl-2-pentanone	C ₆ H ₁₂ O ₂			+
2-Methyl-1,3-cyclohexanedione	C ₇ H ₁₀ O ₂	+		
2-Hepten-4-one	C ₇ H ₁₂ O	+		
2,3-Heptanedione	C ₇ H ₁₂ O ₂	+		
2,4-Dimethyl-3-pentanone	C ₇ H ₁₄ O			+
2-Heptanone	C ₇ H ₁₄ O	+	+	+
3-Heptanone	C ₇ H ₁₄ O			+
4-Ethoxy-2-pentanone	C ₇ H ₁₄ O ₂			+
6-Methyl-3,4-heptadien-2-one	C ₈ H ₁₂ O			
6-Methyl-3,4-heptadien-2-one, <i>cis</i> -				+
6-Methyl-3,4-heptadien-2-one, <i>trans</i> -				+
6-Methyl-5-hepten-2-one	C ₈ H ₁₄ O	+	+	+
1-Octen-3-one	C ₈ H ₁₄ O		+	
2-Octanone	C ₈ H ₁₆ O	+	+	+
3-Octanone	C ₈ H ₁₆ O		+	+
3,5,5-Trimethyl-2-cyclohexene-1,4-dione	C ₉ H ₁₂ O ₂			+
3-Nonen-2-one, <i>trans</i> -	C ₉ H ₁₆ O			+
2-Nonen-4-one, <i>trans</i> -	C ₉ H ₁₆ O			+
2-Nonanone	C ₉ H ₁₈ O	+	+	+
2-Decanone	C ₁₀ H ₂₀ O	+	+	+
2-Undecen-4-one, <i>trans</i> -	C ₁₁ H ₂₀ O			+
2-Undecanone	C ₁₁ H ₂₂ O	+	+	+

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
2-Dodecanone	$C_{12}H_{24}O$			+
2-Tridecanone	$C_{13}H_{26}O$			+
2-Tetradecanone	$C_{14}H_{28}O$			+
<i>Acetals</i>				
Formaldehyde dimethyl acetal	$C_3H_8O_2$	+		
2,4-Dimethyl-1,3-dioxolane	$C_5H_{10}O_2$		+	
5-Hydroxy-2-methyl-1,3-dioxane	$C_5H_{10}O_3$			
5-Hydroxy-2-methyl-1,3-dioxane, <i>cis</i> -			+	
5-Hydroxy-2-methyl-1,3-dioxane, <i>trans</i> -			+	
4-Hydroxymethyl-2-methyl-1,3-dioxolane	$C_5H_{10}O_3$			
4-Hydroxymethyl-2-methyl-1,3-dioxolane, <i>cis</i> -			+	
4-Hydroxymethyl-2-methyl-1,3-dioxolane, <i>trans</i> -			+	
Formaldehyde diethyl acetal	$C_5H_{12}O_2$			+
Acetaldehyde methyl ethyl acetal	$C_5H_{12}O_2$		+	+
2,4,5-Trimethyl-1,3-dioxolane	$C_6H_{12}O_2$		+	+
Acetaldehyde acetyl ethyl acetal	$C_6H_{12}O_3$			+
Acetaldehyde diethyl acetal (Acetal)	$C_6H_{14}O_2$	+	+	+
Acetaldehyde methyl propyl acetal	$C_6H_{14}O_2$		+	
2,4-Dimethyl-5-ethyl-1,3-dioxolane	$C_7H_{14}O_2$		+	
2-Isopropyl-4-methyl-1,3-dioxolane	$C_7H_{14}O_2$		+	
Acrolein diethyl acetal	$C_7H_{14}O_2$			+
Pyruvaldehyde diethyl acetal	$C_7H_{14}O_3$		+	+
Acetaldehyde ethyl propyl acetal	$C_7H_{16}O_2$		+	+
Propionaldehyde diethyl acetal	$C_7H_{16}O_2$			+
Acetaldehyde diallyl acetal	$C_8H_{14}O_2$			+
2-Isobutyl-4-methyl-1,3-dioxolane	$C_8H_{16}O_2$			
2-Isobutyl-4-methyl-1,3-dioxolane, <i>cis</i> -			+	
2-Isobutyl-4-methyl-1,3-dioxolane, <i>trans</i> -			+	
2,3-Butanedione diethyl acetal	$C_8H_{16}O_3$			+
Acetaldehyde ethyl isobutyl acetal	$C_8H_{18}O_2$			+
Acetaldehyde ethyl butyl acetal	$C_8H_{18}O_2$			+
Acetaldehyde dipropyl acetal	$C_8H_{18}O_2$		+	+
Isobutyraldehyde diethyl acetal	$C_8H_{18}O_2$			+
Butyraldehyde diethyl acetal	$C_8H_{18}O_2$			+
Hexanaldehyde dimethyl acetal	$C_8H_{18}O_2$			+
Ethoxyacetaldehyde diethyl acetal	$C_8H_{18}O_3$		+	
2-Ethoxyacetaldehyde diethyl acetal	$C_8H_{18}O_3$			+
2-Pentyl-4-methyl-1,3-dioxolane, <i>trans</i> -	$C_9H_{18}O_2$		+	
Acetaldehyde ethyl 2-methylbutyl acetal	$C_9H_{20}O_2$		+	+
Acetaldehyde ethyl isopentyl acetal	$C_9H_{20}O_2$		+	+
Acetaldehyde ethyl pentyl acetal	$C_9H_{20}O_2$			+
Priopionaldehyde ethyl isobutyl acetal	$C_9H_{20}O_2$			+
Isobutyraldehyde ethyl propyl acetal	$C_9H_{20}O_2$			+
2-Methylbutyraldehyde diethyl acetal	$C_9H_{20}O_2$			+

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
Isovaleraldehyde diethyl acetal	$C_9H_{20}O_2$			+
Valeraldehyde diethyl acetal	$C_9H_{20}O_2$		+	+
3-Ethoxypropionaldehyde diethyl acetal	$C_9H_{20}O_3$			+
Acetaldehyde ethyl 3-hexenyl acetal	$C_{10}H_{20}O_2$			+
Acetaldehyde ethyl hexyl acetal	$C_{10}H_{20}O_2$			+
Acetaldehyde isopentyl propyl acetal	$C_{10}H_{20}O_2$			+
Acetaldehyde diisobutyl acetal	$C_{10}H_{20}O_2$		+	+
Acetaldehyde dibutyl acetal	$C_{10}H_{20}O_2$		+	
Propionaldehyde ethyl isopentyl acetal	$C_{10}H_{20}O_2$			+
Isobutyraldehyde ethyl isobutyl acetal	$C_{10}H_{22}O_2$			+
Hexanaldehyde diethyl acetal	$C_{10}H_{22}O_2$			+
3-Hydroxypropionaldehyde ethyl isopentyl acetal	$C_{10}H_{22}O_3$			+
3-Ethoxy-2-methylpropionaldehyde diethyl acetal	$C_{10}H_{22}O_3$			+
3-Ethoxybutyraldehyde diethyl acetal	$C_{10}H_{22}O_3$			+
Acetaldehyde ethyl benzyl acetal	$C_{11}H_{16}O_2$			+
Acetaldehyde isobutyl isopentyl acetal	$C_{11}H_{24}O_2$		+	+
Acetaldehyde butyl isopentyl acetal	$C_{11}H_{24}O_2$			+
Acetaldehyde butyl pentyl acetal	$C_{11}H_{24}O_2$			+
Propionaldehyde propyl isopentyl acetal	$C_{11}H_{24}O_2$			+
Propionaldehyde diisobutyl acetal	$C_{11}H_{24}O_2$			+
Isobutyraldehyde ethyl isopentyl acetal	$C_{11}H_{24}O_2$			+
Isobutyraldehyde propyl isobutyl acetal	$C_{11}H_{24}O_2$			+
Butyraldehyde ethyl isopentyl acetal	$C_{11}H_{24}O_2$			+
Butyraldehyde ethyl pentyl acetal	$C_{11}H_{24}O_2$			+
Isovaleraldehyde ethyl isobutyl acetal	$C_{11}H_{24}O_2$			+
Isovaleraldehyde dipropyl acetal	$C_{11}H_{24}O_2$			+
Valeraldehyde ethyl isobutyl acetal	$C_{11}H_{24}O_2$			+
Acetaldehyde ethyl phenethyl acetal	$C_{12}H_{18}O_2$		+	+
2-Phenylacetaldehyde diethyl acetal	$C_{12}H_{18}O_2$		+	+
Acetaldehyde di(2-methylbutyl) acetal	$C_{12}H_{26}O_2$		+	+
Acetaldehyde isopentyl 2-methylbutyl acetal	$C_{12}H_{26}O_2$		+	+
Acetaldehyde diisopentyl acetal	$C_{12}H_{26}O_2$		+	+
Acetaldehyde isopentyl pentyl acetal	$C_{12}H_{26}O_2$			+
Isobutyraldehyde propyl isopentyl acetal	$C_{12}H_{26}O_2$			+
Isobutyraldehyde diisobutyl acetal	$C_{12}H_{26}O_2$			+
Isovaleraldehyde ethyl isopentyl acetal	$C_{12}H_{26}O_2$			+
Isovaleraldehyde propyl isobutyl acetal	$C_{12}H_{26}O_2$			+
Valeraldehyde ethyl pentyl acetal	$C_{12}H_{26}O_2$			+
3-Ethoxypropionaldehyde ethyl isopentyl acetal	$C_{12}H_{26}O_3$			+
Acetaldehyde isopentyl hexyl acetal	$C_{13}H_{28}O_2$		+	
Isobutyraldehyde isobutyl isopentyl acetal	$C_{13}H_{28}O_2$			+
Isovaleraldehyde isopentyl propyl acetal	$C_{13}H_{28}O_2$			+
Isovaleraldehyde diisobutyl acetal	$C_{13}H_{28}O_2$			+
Valeraldehyde diisobutyl acetal	$C_{13}H_{28}O_2$			+
Acetaldehyde dihexyl acetal	$C_{14}H_{30}O_2$		+	

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
Isobutyraldehyde diisopentyl acetal	$C_{14}H_{30}O_2$			+
Isovaleraldehyde isobutyl isopentyl acetal	$C_{14}H_{30}O_2$			+
Ethoxyacetaldehyde dipentyl acetal	$C_{14}H_{30}O_3$		+	
Acetaldehyde 2-methylbutyl phenethyl acetal	$C_{15}H_{24}O_2$		+	
Acetaldehyde isopentyl phenethyl acetal	$C_{15}H_{24}O_2$		+	
Isovaleraldehyde diisopentyl acetal	$C_{15}H_{32}O_2$			+
Hexoxyacetaldehyde dipentyl acetal	$C_{18}H_{38}O_3$		+	
<i>Aliphatic monocarboxylic acids</i>				
Formic acid	CH_2O_2	+	+	
Acetic acid	$C_2H_4O_2$	+	+	+
Propionic acid	$C_3H_6O_2$	+	+	+
Crotonic acid	$C_4H_6O_2$	+		
Isobutyric acid	$C_4H_8O_2$	+	+	+
Butyric acid	$C_4H_8O_2$	+	+	+
Pentenoic acid	$C_5H_8O_2$	+		
2-Methylbutyric acid	$C_5H_{10}O_2$	+	+	+
Isovaleric acid	$C_5H_{10}O_2$	+	+	+
Valeric acid	$C_5H_{10}O_2$	+	+	+
3-Ethoxypropionic acid	$C_5H_{10}O_3$			+
Sorbic acid	$C_6H_8O_2$		+	
4-Methyl-3-pentenoic acid	$C_6H_{10}O_2$	+	+	
Hexenoic acid	$C_6H_{10}O_2$	+	+	
2-Hexenoic acid	$C_6H_{10}O_2$	+		
3-Hexenoic acid	$C_6H_{10}O_2$	+	+	
3-Hexenoic acid, <i>cis</i> -			+	
4-Methylvaleric acid	$C_6H_{12}O_2$	+		+
Hexanoic acid	$C_6H_{12}O_2$	+	+	+
Heptenoic acid	$C_7H_{12}O_2$	+		+
2-Heptenoic acid	$C_7H_{12}O_2$	+		
2-Ethyl-3-methylbutanoic acid	$C_7H_{14}O_2$			+
2-Methylhexanoic acid	$C_7H_{14}O_2$			+
Heptanoic acid	$C_7H_{14}O_2$	+	+	+
2-Octenoic acid	$C_8H_{14}O_2$	+		
2-Ethylhexanoic acid	$C_8H_{16}O_2$		+	
6-Methylheptanoic acid	$C_8H_{16}O_2$			+
Octanoic acid	$C_8H_{16}O_2$	+	+	+
2-Nonenoic acid	$C_9H_{16}O_2$	+		
Nonanoic acid	$C_9H_{18}O_2$	+	+	+
3,7-Dimethyl-2,6-octadienoic acid	$C_{10}H_{16}O_2$		+	
Decadienoic acid	$C_{10}H_{16}O_2$	+		
4,8-Decadienoic acid	$C_{10}H_{16}O_2$	+		
Decenoic acid	$C_{10}H_{18}O_2$	+		
4-Decenoic acid	$C_{10}H_{18}O_2$	+		
9-Decenoic acid	$C_{10}H_{18}O_2$		+	

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
Decanoic acid	$C_{10}H_{20}O_2$	+	+	+
10-Undecenoic acid	$C_{11}H_{20}O_2$		+	+
9-Methyldecanoic acid	$C_{11}H_{22}O_2$	+		
Undecanoic acid	$C_{11}H_{22}O_2$	+	+	+
Dodecenoic acid	$C_{12}H_{22}O_2$	+		
Lauric acid	$C_{12}H_{24}O_2$	+	+	+
Methylauric acid	$C_{13}H_{26}O_2$	+		
Tridecanoic acid	$C_{13}H_{26}O_2$	+	+	+
Tetradecenoic acid	$C_{14}H_{26}O_2$	+		
Myristic acid	$C_{14}H_{28}O_2$	+	+	+
Pentadecanoic acid	$C_{15}H_{30}O_2$	+	+	+
9-Hexadecenoic acid	$C_{16}H_{30}O_2$	+	+	+
Palmitic acid	$C_{16}H_{32}O_2$	+	+	+
Heptadecanoic acid	$C_{17}H_{34}O_2$	+	+	+
Linolenic acid	$C_{18}H_{30}O_2$	+		+
Linoleic acid	$C_{18}H_{32}O_2$	+		+
Oleic acid	$C_{18}H_{34}O_2$	+	+	+
Stearic acid	$C_{18}H_{36}O_2$	+	+	+
Docosanoic acid	$C_{22}H_{44}O_2$	+		
Hexacosanoic acid	$C_{26}H_{52}O_2$	+		
<i>Aliphatic monobasic hydroxy acids</i>				
Glycolic acid	$C_2H_4O_3$	+	+	
Lactic acid	$C_3H_6O_3$	+	+	+
D-Lactic acid		+	+	
L-Lactic acid		+	+	
2-Methylactic acid	$C_4H_8O_3$		+	
2-Hydroxybutyric acid	$C_4H_8O_3$		+	
2-Hydroxy-2-methylbutyric acid	$C_5H_{10}O_3$		+	
2-Hydroxy-3-methylbutyric acid	$C_5H_{10}O_3$	+	+	
2,3-Dihydroxy-2-methylbutyric acid	$C_5H_{10}O_4$		+	
2,3-Dihydroxy-3-methylbutyric acid	$C_5H_{10}O_4$		+	
2-Hydroxy-3-methylvaleric acid	$C_6H_{12}O_3$	+	+	
D-2-Hydroxy-3-methylvaleric acid			+	
L-2-Hydroxy-3-methylvaleric acid			+	
Hydroxy-4-methylvaleric acid	$C_6H_{12}O_3$	+	+	
2-Hydroxyhexanoic acid	$C_6H_{12}O_3$		+	
2-Hydroxyheptanoic acid	$C_7H_{14}O_3$	+		
2-Hydroxyoctanoic acid	$C_8H_{16}O_3$	+		
3-Hydroxyoctanoic acid	$C_8H_{16}O_3$	+	+	
3-Hydroxydecanoic acid	$C_{10}H_{20}O_3$	+		
2-Hydroxylauric acid	$C_{12}H_{24}O_3$		+	
9,10,11-Trihydroxy-12-octadecenoic acid, <i>trans</i> -	$C_{18}H_{34}O_5$	+		
9,10,13-Trihydroxy-11-octadecenoic acid, <i>trans</i> -	$C_{18}H_{34}O_5$	+		
9,12,13-Trihydroxy-11-octadecenoic acid, <i>trans</i> -	$C_{18}H_{34}O_5$	+		

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
<i>Aldonic and uronic acids</i>				
Ascorbic acid	C ₆ H ₈ O ₆		+	
arabino-Hexulosonic acid (2-Ketogluconic acid)	C ₆ H ₁₀ O ₇	+		
Glucuronic acid	C ₆ H ₁₀ O ₇	+	+	
Galacturonic acid	C ₆ H ₁₀ O ₇	+	+	
Galactaric acid	C ₆ H ₁₀ O ₈		+	
Gluconic acid	C ₆ H ₁₂ O ₇	+	+	
<i>Aliphatic monobasic oxo acids</i>				
Glyoxylic acid	C ₂ H ₂ O ₃	+	+	
Glyoxylic acid, <i>syn</i> -		+		
Glyoxylic acid, <i>anti</i> -		+		
Pyruvic acid	C ₃ H ₄ O ₃	+	+	
Pyruvic acid, <i>syn</i> -		+		
Pyruvic acid, <i>anti</i> -		+		
2-Oxobutyric acid	C ₄ H ₆ O ₃	+		
Acetoacetic acid	C ₄ H ₆ O ₃		+	
3-Methyl-2-oxobutyric acid	C ₅ H ₈ O ₃	+		
Levulinic acid	C ₅ H ₈ O ₃	+	+	
2-Hydroxy-2-methylacetoacetic acid	C ₅ H ₈ O ₄	+		
3-Methyl-2-oxovaleric acid	C ₆ H ₁₀ O ₃	+		
4-Methyl-2-oxovaleric acid	C ₆ H ₁₀ O ₃	+	+	
2-Oxohexanoic acid	C ₆ H ₁₀ O ₃	+	+	
5-Oxohexanoic acid	C ₆ H ₁₀ O ₃	+		
2-Ethyl-2-hydroxyacetoacetic acid	C ₆ H ₁₀ O ₄	+		
7-Oxoheptanoic acid	C ₇ H ₁₂ O ₃	+		
<i>Aliphatic di- and tricarboxylic acids</i>				
Oxalic acid	C ₂ H ₂ O ₄	+	+	
Mesoxalic acid	C ₂ H ₂ O ₅		+	
Malonic acid	C ₃ H ₄ O ₄	+	+	
Fumaric acid	C ₄ H ₄ O ₄	+	+	
Oxalacetic acid	C ₄ H ₄ O ₅	+	+	
Succinic acid	C ₄ H ₆ O ₄	+	+	
Malic acid	C ₄ H ₆ O ₅	+	+	
Tartaric acid	C ₄ H ₆ O ₆	+	+	
Mesaconic acid	C ₅ H ₆ O ₄	+	+	
Citraconic acid	C ₅ H ₆ O ₄	+	+	
Methylenesuccinic acid	C ₅ H ₆ O ₄		+	
Glutaconic acid	C ₅ H ₆ O ₄		+	
2-Oxoglutaric acid	C ₅ H ₆ O ₅	+	+	
Methylsuccinic acid	C ₅ H ₈ O ₄		+	
Glutaric acid	C ₅ H ₈ O ₄	+	+	
2-Methylmalic acid	C ₅ H ₈ O ₅	+	+	
2-Hydroxyglutaric acid	C ₅ H ₈ O ₅	+	+	

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
1-Propene-1,2,3-tricarboxylic acid	C ₆ H ₆ O ₆	+	+	
1-Propene-1,2,3-tricarboxylic acid, <i>cis</i> -			+	
1-Oxo-1,2,3-propanetricarboxylic acid	C ₆ H ₆ O ₇	+		
1,2,3-Propanetricarboxylic acid	C ₆ H ₈ O ₆		+	
Isocitric acid	C ₆ H ₈ O ₇	+	+	
Citric acid	C ₆ H ₈ O ₇	+	+	
3-Methylglutaric acid	C ₆ H ₁₀ O ₄		+	
Adipic acid	C ₆ H ₁₀ O ₄		+	
Galactaric acid	C ₆ H ₁₀ O ₈		+	
Pimelic acid	C ₇ H ₁₂ O ₄	+	+	
2-Isopropylmalic acid	C ₇ H ₁₂ O ₅	+	+	
Suberic acid	C ₈ H ₁₄ O ₄	+	+	
3-Ethylheptanedioic acid	C ₉ H ₁₆ O ₄			+
Azelaic acid	C ₉ H ₁₆ O ₄	+	+	
Sebacic acid	C ₁₀ H ₁₈ O ₄	+	+	
Undecanedioic acid	C ₁₁ H ₂₀ O ₄	+		
Dodecanedioic acid	C ₁₂ H ₂₂ O ₄	+		
<i>Esters of aliphatic monocarboxylic acids</i>				
Methyl formate	C ₂ H ₄ O ₂	+	+	+
Ethyl formate	C ₃ H ₆ O ₂	+	+	+
Methyl acetate	C ₃ H ₆ O ₂	+	+	+
Vinyl acetate (IARC, 1986b, 1987a)	C ₄ H ₆ O ₂			+
Isopropyl formate	C ₄ H ₈ O ₂		+	
Propyl formate	C ₄ H ₈ O ₂		+	
Ethyl acetate	C ₄ H ₈ O ₂	+	+	+
Methyl propionate	C ₄ H ₈ O ₂		+	+
Acetonyl acetate	C ₅ H ₈ O ₃	+		
Isobutyl formate	C ₅ H ₁₀ O ₂	+		+
Butyl formate	C ₅ H ₁₀ O ₂		+	
Isopropyl acetate	C ₅ H ₁₀ O ₂	+	+	+
Propyl acetate	C ₅ H ₁₀ O ₂	+	+	+
Ethyl propionate	C ₅ H ₁₀ O ₂	+	+	+
Methyl isobutyrate	C ₅ H ₁₀ O ₂		+	+
Methyl butyrate	C ₅ H ₁₀ O ₂		+	+
1,3-Propanediol monoacetate	C ₅ H ₁₀ O ₃		+	
Furfuryl formate	C ₆ H ₆ O ₃	+		
Ethyl methacrylate	C ₆ H ₁₀ O ₂		+	
Ethyl 2-butenolate	C ₆ H ₁₀ O ₂		+	
Ethyl 2-butenolate, <i>trans</i> -			+	
2-Methylbutyl formate	C ₆ H ₁₂ O ₂		+	
Isopentyl formate	C ₆ H ₁₂ O ₂	+	+	+
Pentyl formate	C ₆ H ₁₂ O ₂			+
<i>tert</i> -Butyl acetate	C ₆ H ₁₂ O ₂			+
Isobutyl acetate	C ₆ H ₁₂ O ₂	+	+	+

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
Butyl acetate	$C_6H_{12}O_2$	+	+	+
<i>sec</i> -Butyl acetate	$C_6H_{12}O_2$	+		+
Isopropyl propionate	$C_6H_{12}O_2$		+	
Propyl propionate	$C_6H_{12}O_2$		+	+
Ethyl isobutyrate	$C_6H_{12}O_2$	+	+	+
Ethyl butyrate	$C_6H_{12}O_2$	+	+	+
Methyl valerate	$C_6H_{12}O_2$		+	
Ethoxyethyl acetate	$C_6H_{12}O_3$			+
2-Butanediol monoacetate	$C_6H_{12}O_3$		+	
2-Butanediol monoacetate, <i>threo</i> -			+	
2-Butanediol monoacetate, <i>erythro</i> -			+	
Furfuryl acetate	$C_7H_8O_3$	+		+
Methyl 2,4-hexadienoate	$C_7H_{10}O_2$		+	
Hexenyl formate	$C_7H_{12}O_2$			+
Methyl hexenoate	$C_7H_{12}O_2$	+		
Isopentyl acetate	$C_7H_{14}O_2$	+	+	+
2-Methylbutyl acetate	$C_7H_{14}O_2$		+	
Pentyl acetate	$C_7H_{14}O_2$	+	+	+
1-Methylbutyl acetate	$C_7H_{14}O_2$		+	
Isobutyl propionate	$C_7H_{14}O_2$		+	+
<i>sec</i> -Butyl propionate	$C_7H_{14}O_2$		+	
<i>tert</i> -Butyl propionate	$C_7H_{14}O_2$			+
Butyl propionate	$C_7H_{14}O_2$			+
Isopropyl isobutyrate	$C_7H_{14}O_2$		+	
Isopropyl butyrate	$C_7H_{14}O_2$		+	
Propyl butyrate	$C_7H_{14}O_2$		+	+
Ethyl 2-methylbutyrate	$C_7H_{14}O_2$	+	+	+
Ethyl isovalerate	$C_7H_{14}O_2$	+	+	+
Ethyl valerate	$C_7H_{14}O_2$		+	+
Methyl 3-methylvalerate	$C_7H_{14}O_2$		+	
Methyl hexanoate	$C_7H_{14}O_2$	+	+	+
Ethyl 3-ethoxypropionate	$C_7H_{14}O_3$			+
Triethyl <i>ortho</i> -formate	$C_7H_{16}O_3$		+	+
Benzyl formate	$C_8H_8O_2$			+
Ethyl sorbate	$C_8H_{12}O_2$		+	+
Cyclohexyl acetate	$C_8H_{14}O_2$		+	
2-Hexenyl acetate, <i>trans</i> -	$C_8H_{14}O_2$			+
3-Hexenyl acetate	$C_8H_{14}O_2$		+	
3-Hexenyl acetate, <i>cis</i> -			+	+
3-Hexenyl acetate, <i>trans</i> -			+	+
Ethyl 4-methyl-3-pentenoate	$C_8H_{14}O_2$		+	
Ethyl hexenoate	$C_8H_{14}O_2$	+		
Ethyl 2-hexenoate	$C_8H_{14}O_2$		+	
Ethyl 2-hexenoate, <i>trans</i> -				+
Ethyl 3-hexenoate, <i>cis</i> -	$C_8H_{14}O_2$	+	+	

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
Methyl 4-methyl-2-hexenoate	$C_8H_{14}O_2$	+		
Methyl heptenoate	$C_8H_{14}O_2$	+		
Heptyl formate	$C_8H_{16}O_2$		+	
Hexyl acetate	$C_8H_{16}O_2$	+	+	+
2-Methylbutyl propionate	$C_8H_{16}O_2$		+	
Isopentyl propionate	$C_8H_{16}O_2$	+	+	+
Pentyl propionate	$C_8H_{16}O_2$		+	
Isobutyl isobutyrate	$C_8H_{16}O_2$		+	+
Butyl isobutyrate	$C_8H_{16}O_2$			+
Isobutyl butyrate	$C_8H_{16}O_2$			+
Butyl butyrate	$C_8H_{16}O_2$		+	+
Ethyl hexanoate	$C_8H_{16}O_2$	+	+	+
Methyl heptanoate	$C_8H_{16}O_2$		+	
Diethoxyethyl acetate	$C_8H_{16}O_4$			+
Phenethyl formate	$C_9H_{10}O_2$	+	+	+
Benzyl acetate (IARC, 1986c, 1987a)	$C_9H_{10}O_2$		+	+
Ethyl heptenoate	$C_9H_{16}O_2$	+		+
Heptyl acetate	$C_9H_{18}O_2$	+	+	+
2-Methylbutyl isobutyrate	$C_9H_{18}O_2$	+	+	
Isopentyl isobutyrate	$C_9H_{18}O_2$	+	+	+
2-Methylbutyl butyrate	$C_9H_{18}O_2$		+	+
Isopentyl butyrate	$C_9H_{18}O_2$	+	+	+
Pentyl butyrate	$C_9H_{18}O_2$	+		
Isobutyl 2-methylbutyrate	$C_9H_{18}O_2$		+	+
Isobutyl isovalerate	$C_9H_{18}O_2$		+	
Isobutyl valerate	$C_9H_{18}O_2$		+	+
Butyl valerate	$C_9H_{18}O_2$		+	
Propyl hexanoate	$C_9H_{18}O_2$		+	+
Ethyl 5-methylhexanoate	$C_9H_{18}O_2$	+		
Ethyl heptanoate	$C_9H_{18}O_2$	+	+	+
Methyl octanoate	$C_9H_{18}O_2$	+	+	+
Phenethyl acetate	$C_{10}H_{12}O_2$	+	+	+
Ethyl phenyl acetate	$C_{10}H_{12}O_2$		+	
Benzyl propionate	$C_{10}H_{12}O_2$			+
4-Hydroxyphenethyl acetate	$C_{10}H_{12}O_3$	+	+	
Octyl acetate	$C_{10}H_{20}O_2$	+	+	+
Hexyl isobutyrate	$C_{10}H_{12}O_2$	+	+	+
Hexyl butyrate	$C_{10}H_{12}O_2$	+	+	+
Isopentyl 2-methylbutyrate	$C_{10}H_{12}O_2$		+	+
Isopentyl isovalerate	$C_{10}H_{12}O_2$	+	+	+
Pentyl isovalerate	$C_{10}H_{12}O_2$	+		
2-Methylbutyl valerate	$C_{10}H_{12}O_2$		+	
Isopentyl valerate	$C_{10}H_{12}O_2$		+	+
Pentyl valerate	$C_{10}H_{12}O_2$		+	
Isobutyl hexanoate	$C_{10}H_{12}O_2$	+	+	+

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
Butyl hexanoate	$C_{10}H_{12}O_2$	+	+	+
Ethyl octanoate	$C_{10}H_{12}O_2$	+	+	+
Methyl nonanoate	$C_{10}H_{12}O_2$		+	
Phenethyl propionate	$C_{11}H_{14}O_2$	+	+	
Methyl 2,4,7-decatrionoate, <i>trans,cis,cis-</i>	$C_{11}H_{16}O_2$			+
<i>trans,trans,cis-</i>				+
Methyl 2,4-decadienoate, <i>trans,cis-</i>	$C_{11}H_{18}O_2$			+
<i>trans,trans-</i>				+
Methyl 4,8-decadienoate	$C_{11}H_{18}O_2$	+		
Ethyl nonenoate	$C_{11}H_{20}O_2$	+		
Methyl 4-decenoate	$C_{11}H_{20}O_2$	+		
Methyl 4-decenoate, <i>cis-</i>	$C_{11}H_{20}O_2$		+	
Nonyl acetate	$C_{11}H_{22}O_2$	+	+	
1-Methylhexyl butyrate	$C_{11}H_{22}O_2$	+		
Hexyl 2-methylbutyrate	$C_{11}H_{22}O_2$			+
Hexyl isovalerate	$C_{11}H_{22}O_2$		+	
Hexyl valerate	$C_{11}H_{22}O_2$		+	+
2-Methylbutyl hexanoate	$C_{11}H_{22}O_2$		+	+
Isopentyl hexanoate	$C_{11}H_{22}O_2$	+	+	+
Pentyl hexanoate	$C_{11}H_{22}O_2$	+	+	+
1-Methylbutyl hexanoate	$C_{11}H_{22}O_2$	+		
Isobutyl heptanoate	$C_{11}H_{22}O_2$			+
Butyl heptanoate	$C_{11}H_{22}O_2$			+
Propyl octanoate	$C_{11}H_{22}O_2$		+	+
Ethyl nonanoate	$C_{11}H_{22}O_2$	+	+	+
Methyl decanoate	$C_{11}H_{22}O_2$	+	+	+
Phenethyl isobutyrate	$C_{12}H_{16}O_2$	+	+	+
Phenethyl butyrate	$C_{12}H_{16}O_2$	+	+	+
Ethyl 2,4,7-decatrionoate, <i>trans,cis,cis-</i>	$C_{12}H_{18}O_2$			+
<i>trans,trans,cis-</i>				+
Ethyl decadienoate	$C_{12}H_{20}O_2$	+	+	
Ethyl 2,4-decadienoate, <i>trans,cis-</i>	$C_{12}H_{20}O_2$			+
<i>trans,trans-</i>				+
Ethyl 4,8-decadienoate	$C_{12}H_{20}O_2$	+		
Ethyl decenoate	$C_{12}H_{22}O_2$	+	+	
Ethyl 2-decenoate, <i>trans-</i>	$C_{12}H_{22}O_2$			+
Ethyl 4-decenoate	$C_{12}H_{22}O_2$	+		
Ethyl 4-decenoate, <i>cis-</i>				+
Ethyl 9-decenoate	$C_{12}H_{22}O_2$	+	+	+
Decyl acetate	$C_{12}H_{24}O_2$		+	+
Octyl butyrate	$C_{12}H_{24}O_2$	+		

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
Hexyl hexanoate	C ₁₂ H ₂₄ O ₂	+	+	+
Isopentyl heptanoate	C ₁₂ H ₂₄ O ₂	+		
Isobutyl octanoate	C ₁₂ H ₂₄ O ₂		+	+
Butyl octanoate	C ₁₂ H ₂₄ O ₂	+	+	+
Ethyl decanoate	C ₁₂ H ₂₄ O ₂	+	+	+
Phenethyl isovalerate	C ₁₃ H ₁₈ O ₂	+		
Phenethyl valerate	C ₁₃ H ₁₈ O ₂		+	
Propyl 2,4-decadienoate, <i>trans,cis</i> -	C ₁₃ H ₂₂ O ₂			+
Methyl 2,6-dodecadienoate, <i>trans,cis</i> -	C ₁₃ H ₂₂ O ₂			+
Heptyl hexanoate	C ₁₃ H ₂₆ O ₂		+	
Hexyl heptanoate	C ₁₃ H ₂₆ O ₂		+	+
2-Methylbutyl octanoate	C ₁₃ H ₂₆ O ₂	+	+	+
Isopentyl octanoate	C ₁₃ H ₂₆ O ₂	+	+	+
Pentyl octanoate	C ₁₃ H ₂₆ O ₂		+	
Isobutyl nonanoate	C ₁₃ H ₂₆ O ₂			+
Propyl decanoate	C ₁₃ H ₂₆ O ₂		+	+
Ethyl undecanoate	C ₁₃ H ₂₆ O ₂		+	+
Methyl laurate	C ₁₃ H ₂₆ O ₂		+	+
Phenethyl hexenoate	C ₁₄ H ₁₈ O ₂	+		
Phenethyl hexanoate	C ₁₄ H ₂₀ O ₂	+	+	+
Butyl 2,4-decadienoate, <i>trans,cis</i> -	C ₁₄ H ₂₄ O ₂			+
Ethyl dodecadienoate	C ₁₄ H ₂₄ O ₂			+
Ethyl 2,6-dodecadienoate, <i>trans,cis</i> -	C ₁₄ H ₂₄ O ₂			+
Isobutyl decenoate	C ₁₄ H ₂₆ O ₂		+	
Ethyl dodecenoate	C ₁₄ H ₂₆ O ₂			+
Ethyl 2-dodecenoate, <i>trans</i> -	C ₁₄ H ₂₆ O ₂			+
Ethyl 6-dodecenoate, <i>cis</i> -	C ₁₄ H ₂₆ O ₂			+
Dodecyl acetate	C ₁₄ H ₂₈ O ₂			+
Octyl hexanoate	C ₁₄ H ₂₈ O ₂	+		
1-Methylheptyl hexanoate	C ₁₄ H ₂₈ O ₂	+		
Hexyl octanoate	C ₁₄ H ₂₈ O ₂	+	+	+
Isopentyl nonanoate	C ₁₄ H ₂₈ O ₂	+		+
Isobutyl decanoate	C ₁₄ H ₂₈ O ₂		+	+
Butyl decanoate	C ₁₄ H ₂₈ O ₂		+	
Ethyl laurate	C ₁₄ H ₂₈ O ₂	+	+	+
Methyl 5,8-tetradecadienoate, <i>cis,cis</i> -	C ₁₅ H ₂₆ O ₂			+
2-Methylbutyl 9-decenoate	C ₁₅ H ₂₈ O ₂		+	
Isopentyl decenoate	C ₁₅ H ₂₈ O ₂		+	
Isopentyl 4-decenoate	C ₁₅ H ₂₈ O ₂	+		
Isopentyl 9-decenoate	C ₁₅ H ₂₈ O ₂		+	
2-Methylbutyl decanoate	C ₁₅ H ₃₀ O ₂	+	+	+
Isopentyl decanoate	C ₁₅ H ₃₀ O ₂	+	+	+
Pentyl decanoate	C ₁₅ H ₃₀ O ₂			+
Propyl laurate	C ₁₅ H ₃₀ O ₂		+	+
Methyl myristate	C ₁₅ H ₃₀ O ₂			+

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
Phenethyl octanoate	$C_{16}H_{24}O_2$	+	+	+
Ethyl 5,8-tetradecadienoate, <i>cis,cis</i> -	$C_{16}H_{28}O_2$			+
Hexyl decenoate	$C_{16}H_{30}O_2$		+	
Ethyl 5-tetradecenoate, <i>cis</i> -	$C_{16}H_{30}O_2$			+
Hexyl decanoate	$C_{16}H_{32}O_2$	+	+	
Isopentyl undecanoate	$C_{16}H_{32}O_2$			+
Isobutyl laurate	$C_{16}H_{32}O_2$	+	+	+
Ethyl myristate	$C_{16}H_{32}O_2$	+	+	+
2-Methylbutyl laurate	$C_{17}H_{34}O_2$		+	+
Isopentyl laurate	$C_{17}H_{34}O_2$	+	+	+
Isobutyl tridecanoate	$C_{17}H_{34}O_2$			+
Isopropyl myristate	$C_{17}H_{34}O_2$			+
Ethyl pentadecanoate	$C_{17}H_{34}O_2$		+	+
Methyl palmitate	$C_{17}H_{34}O_2$			+
Phenethyl decanoate	$C_{18}H_{28}O_2$			+
Ethyl 9-hexadecenoate	$C_{18}H_{34}O_2$			+
Isopentyl tridecanoate	$C_{18}H_{36}O_2$			+
Isobutyl myristate	$C_{18}H_{36}O_2$			+
Ethyl palmitate	$C_{18}H_{36}O_2$		+	+
Methyl linoleate	$C_{19}H_{34}O_2$			+
Methyl oleate	$C_{19}H_{36}O_2$			+
2-Methylbutyl myristate	$C_{19}H_{38}O_2$		+	+
Isopentyl myristate	$C_{19}H_{38}O_2$		+	+
Propyl palmitate	$C_{19}H_{38}O_2$			+
Ethyl heptadecanoate	$C_{19}H_{38}O_2$			+
Ethyl linolenate	$C_{20}H_{34}O_2$	+		+
Ethyl linoleate	$C_{20}H_{36}O_2$	+		+
Ethyl oleate	$C_{20}H_{38}O_2$	+		+
Hexyl myristate	$C_{20}H_{40}O_2$			+
Isopentyl pentadecanoate	$C_{20}H_{40}O_2$			+
Isobutyl palmitate	$C_{20}H_{40}O_2$			+
Ethyl stearate	$C_{20}H_{40}O_2$		+	+
2-Methylbutyl palmitate	$C_{21}H_{42}O_2$		+	+
Isopentyl palmitate	$C_{21}H_{42}O_2$		+	+
Ethyl nonadecanoate	$C_{21}H_{42}O_2$			+
Isobutyl stearate	$C_{22}H_{44}O_2$			+
Ethyl eicosanoate	$C_{22}H_{44}O_2$			+
Ethyl heneicosanoate	$C_{23}H_{46}O_2$			+
Isobutyl eicosanoate	$C_{24}H_{48}O_2$			+
Ethyl docosanoate	$C_{24}H_{48}O_2$			+
Ethyl tricosanoate	$C_{25}H_{50}O_2$			+
Ethyl tetracosanoate	$C_{26}H_{52}O_2$			+
<i>Esters of aliphatic monobasic hydroxy and oxo acids</i>				
Methyl lactate	$C_4H_8O_3$		+	

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
Ethyl pyruvate	$C_5H_8O_3$		+	+
Ethyl lactate	$C_5H_{10}O_3$	+	+	+
Ethyl hydracrylate	$C_5H_{10}O_3$		+	
Ethyl acetoacetate	$C_6H_{10}O_3$		+	
Propyl lactate	$C_6H_{12}O_3$		+	
Ethyl 2-hydroxybutyrate	$C_6H_{12}O_3$		+	+
Ethyl 3-hydroxybutyrate	$C_6H_{12}O_3$		+	+
Ethyl 4-hydroxybutyrate	$C_6H_{12}O_3$		+	
Ethyl levulinate	$C_7H_{12}O_3$	+	+	+
Isobutyl lactate	$C_7H_{14}O_3$		+	+
Butyl lactate	$C_7H_{14}O_3$			+
Ethyl 2-hydroxy-2-methylbutyrate	$C_7H_{14}O_3$		+	
Ethyl 2-hydroxy-3-methylbutyrate	$C_7H_{14}O_3$		+	+
Ethyl 4-hydroxyvalerate	$C_7H_{14}O_3$		+	
Isopentyl lactate	$C_8H_{16}O_3$	+	+	+
Ethyl 2-hydroxy-3-methylvalerate	$C_8H_{16}O_3$		+	+
Ethyl 2-hydroxy-4-methylvalerate	$C_8H_{16}O_3$		+	+
2,4-Hexadienyl lactate, <i>trans,trans</i> -	$C_9H_{14}O_3$		+	
3-Hexenyl lactate, <i>cis</i> -	$C_9H_{16}O_3$			+
Hexyl lactate	$C_9H_{18}O_3$		+	+
Methyl 3-hydroxyoctanoate	$C_9H_{18}O_3$			+
Ethyl 2,2-diethoxypropionate	$C_9H_{18}O_4$		+	+
Ethyl 3-hydroxyoctanoate	$C_{10}H_{20}O_3$			+
<i>Esters of aliphatic di- and tricarboxylic acids</i>				
Diethyl oxalate	$C_6H_{10}O_4$		+	+
Ethyl hydrogen succinate	$C_6H_{10}O_4$	+	+	+
Dimethyl malate	$C_6H_{10}O_5$		+	
Ethyl hydrogen malate	$C_6H_{10}O_5$		+	
Ethyl hydrogen tartrate	$C_6H_{10}O_6$		+	
Diethyl malonate	$C_7H_{12}O_4$		+	+
Ethyl methyl succinate	$C_7H_{12}O_4$		+	+
Propyl hydrogen succinate	$C_7H_{12}O_4$		+	
Ethyl hydrogen glutarate	$C_7H_{12}O_4$		+	
Ethyl methyl malate	$C_7H_{12}O_5$		+	
Ethyl hydrogen 2-methylmalate	$C_7H_{12}O_5$		+	
Diethyl fumarate	$C_8H_{12}O_4$		+	+
Diethyl maleate	$C_8H_{12}O_4$		+	
Ethyl dihydrogen citrate	$C_8H_{12}O_7$			+
Diethyl succinate	$C_8H_{14}O_4$	+	+	+
Isobutyl hydrogen succinate	$C_8H_{14}O_4$		+	
Butyl hydrogen succinate	$C_8H_{14}O_4$		+	
Ethyl methyl glutarate	$C_8H_{14}O_4$			+
Diethyl malate	$C_8H_{14}O_5$		+	+
Diethyl tartrate	$C_8H_{14}O_6$		+	+

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
Ethyl propyl succinate	$C_9H_{16}O_4$		+	+
Isopentyl hydrogen succinate	$C_9H_{16}O_4$		+	
Diethyl methylsuccinate	$C_9H_{16}O_4$		+	+
Diethyl glutarate	$C_9H_{16}O_4$		+	+
Diethyl 2-methylmalate	$C_9H_{16}O_5$		+	
Ethyl hydrogen 2-isopropylmalate	$C_9H_{16}O_5$		+	
Diethyl 2-hydroxyglutarate	$C_9H_{16}O_5$		+	
Ethyl isobutyl succinate	$C_{10}H_{18}O_4$		+	+
Butyl ethyl succinate	$C_{10}H_{18}O_4$			+
Dipropyl succinate	$C_{10}H_{18}O_4$		+	
Diethyl adipate	$C_{10}H_{18}O_4$			+
Ethyl 2-methylbutyl succinate	$C_{11}H_{20}O_4$		+	
Ethyl isopentyl succinate	$C_{11}H_{20}O_4$		+	+
Ethyl pentyl succinate	$C_{11}H_{20}O_4$			+
Ethyl hydrogen azelate	$C_{11}H_{20}O_4$		+	
Ethyl hexyl succinate	$C_{12}H_{22}O_4$			+
Diethyl suberate	$C_{12}H_{22}O_4$			+
Diethyl azelate	$C_{13}H_{24}O_4$			+
Diisopentyl succinate	$C_{14}H_{26}O_4$		+	+
Tributyl 1-propene-1,2,3-tricarboxylate	$C_{18}H_{30}O_6$		+	
<i>Amines and amides</i>				
Ammonia	H_3N	+		
Methylamine	CH_5N	+	+	
<i>N</i> -Nitrosodimethylamine (IARC, 1978, 1987a)	$C_2H_6N_2O$	+	+	+
Ethylamine	C_2H_7N	+	+	
Dimethylamine	C_2H_7N	+	+	
2-Aminoethanol	C_2H_7NO	+	+	
Ethylenediamine	$C_2H_8N_2$		+	
<i>N,N</i> -Dimethylformamide	C_3H_7NO	+		
<i>N</i> -Methylacetamide	C_3H_7NO	+		
Ethyl carbamate (Urethane) (IARC, 1974, 1987a)	$C_3H_7NO_2$		+	+
Trimethylamine	C_3H_9N	+		
Isopropylamine	C_3H_9N	+	+	
Propylamine	C_3H_9N	+	+	
3-Amino-1-propanol	C_3H_9NO	+	+	
1,3-Propanediamine	$C_3H_{10}N_2$	+	+	
<i>N</i> -Nitrosopyrrolidine (IARC, 1978, 1987a)	$C_4H_8N_2O$	+		
<i>N,N</i> -Dimethylacetamide	C_4H_9NO	+		
<i>N</i> -Ethylacetamide	C_4H_9NO	+	+	
<i>N</i> -Nitrosodiethylamine (IARC, 1978, 1987a)	$C_4H_{10}N_2O$	+	+	+
Isobutylamine	$C_4H_{11}N$	+	+	
Butylamine	$C_4H_{11}N$	+	+	
<i>sec</i> -Butylamine	$C_4H_{11}N$	+		
1,4-Butanediamine	$C_4H_{12}N_2$	+	+	

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
<i>N</i> -Nitrosoproline (IARC, 1978, 1987a)	C ₅ H ₈ N ₂ O ₃	+		
Betaine	C ₅ H ₁₁ NO ₂		+	
Isopentylamine	C ₅ H ₁₃ N	+	+	
Pentylamine	C ₅ H ₁₃ N	+	+	
1,5-Pentanediamine	C ₅ H ₁₄ N ₂	+	+	
Choline	C ₅ H ₁₅ NO ₂	+		
2-(Diacetylamino)ethanol	C ₆ H ₁₁ NO ₃		+	
<i>N</i> -Isobutylacetamide	C ₆ H ₁₃ NO		+	
<i>N</i> -[3-(Methylthio)propyl]acetamide	C ₆ H ₁₃ NOS		+	
<i>N</i> -Nitrosodi- <i>n</i> -propylamine (IARC, 1978, 1987a)	C ₆ H ₁₄ N ₂ O		+	+
<i>N,N</i> -Dimethylbutylamine	C ₆ H ₁₅ N	+		
Hexylamine	C ₆ H ₁₅ N	+	+	
<i>para</i> -(Aminomethyl)phenol	C ₇ H ₉ NO	+		
<i>N</i> -Furfurylacetamide	C ₇ H ₉ NO ₂	+		
<i>N</i> -Methyl- <i>N</i> -butylacetamide	C ₇ H ₁₅ NO		+	
<i>N</i> -(2-Methylbutyl)acetamide	C ₇ H ₁₅ NO	+	+	
<i>N</i> -Isopentylacetamide	C ₇ H ₁₅ NO	+	+	
Choline acetate	C ₇ H ₁₇ NO ₃		+	
<i>N</i> -(3-Aminopropyl)-1,4-butanediamine	C ₇ H ₁₉ N ₃	+	+	
Phenylacetone nitrile	C ₈ H ₇ N			+
2'-Aminoacetophenone	C ₈ H ₉ NO	+		
Methyl anthranilate	C ₈ H ₉ NO ₂		+	
Phenethylamine	C ₈ H ₁₁ N	+	+	
<i>para</i> -(2-Aminoethyl)phenol	C ₈ H ₁₁ NO	+	+	
Diisobutylamine	C ₈ H ₁₉ N	+		
<i>N</i> -Methylphenylethylamine	C ₉ H ₁₃ N	+	+	
<i>para</i> -[2-(Methylamino)]phenol	C ₉ H ₁₃ NO	+		
Tripropylamine	C ₉ H ₂₁ N	+		
<i>N</i> -Phenethylacetamide	C ₁₀ H ₁₃ NO	+	+	
<i>para</i> -[2-(Dimethylamino)ethyl]phenol	C ₁₀ H ₁₅ NO	+		
<i>N,N</i> -Bis(3-aminopropyl)-1,4-butanediamine	C ₁₀ H ₂₆ N ₄	+		
2-Amino-4-octadecene-1,3-diol	C ₁₈ H ₃₇ NO ₂		+	
<i>N-Heterocyclics</i>				
Thiazole	C ₃ H ₃ NS	+		+
Pyrazine	C ₄ H ₄ N ₂	+		
Uracil	C ₄ H ₄ N ₂ O ₂	+	+	
Pyrrole	C ₄ H ₅ N	+		
Cytosine	C ₄ H ₅ N ₃ O	+	+	
2-Pyrrolidone	C ₄ H ₇ NO	+		
Pyrrolidine	C ₄ H ₉ N	+	+	
Hypoxanthine	C ₅ H ₄ N ₄ O	+	+	
Xanthine	C ₅ H ₄ N ₄ O ₂	+	+	
Pyridine	C ₅ H ₅ N	+		+
Pyrrole-2-carboxaldehyde	C ₅ H ₅ NO	+		

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
2-Acetylthiazole	C ₅ H ₅ NOS	+		
Adenine	C ₅ H ₅ N ₅	+	+	
Guanine	C ₅ H ₅ N ₅ O	+		
Methylpyrazine	C ₅ H ₆ N ₂	+		+
Thymine	C ₅ H ₆ N ₂ O ₂	+	+	
1-Methylpyrrole	C ₅ H ₇ N	+		
2-Methylpyrrole	C ₅ H ₇ N	+		
5-Oxoproline	C ₅ H ₇ NO ₃	+		
1-Methyl-2-pyrrolidone	C ₅ H ₉ NO	+		
Histamine	C ₅ H ₉ N ₃	+	+	
Piperidine	C ₅ H ₁₁ N		+	
Nicotinic acid	C ₆ H ₅ NO ₂		+	
Picoline	C ₆ H ₇ N		+	
α-Picoline	C ₆ H ₇ N			+
β-Picoline	C ₆ H ₇ N			+
γ-Picoline	C ₆ H ₇ N			+
1-Methylpyrrole-2-carboxaldehyde	C ₆ H ₇ NO			+
5-Methylpyrrole-2-carboxaldehyde	C ₆ H ₇ NO	+		
Methyl 1-pyrrolyl ketone	C ₆ H ₇ NO	+		
Methyl 2-pyrrolyl ketone	C ₆ H ₇ NO	+		
4-Methyl-4-vinylthiazole	C ₆ H ₇ NS			+
2,3-Dimethylpyrazine	C ₆ H ₈ N ₂	+		+
2,5-Dimethylpyrazine	C ₆ H ₈ N ₂	+		+
2,6-Dimethylpyrazine	C ₆ H ₈ N ₂	+		+
Ethylpyrazine	C ₆ H ₈ N ₂	+		+
5-Hydroxyethyl-4-methylthiazole	C ₆ H ₉ NOS	+		
4-Methyl-5-(β-hydroxyethyl)thiazole	C ₆ H ₉ NOS			+
Histidine	C ₆ H ₉ N ₃ O ₂		+	
2-Benzothiazolol	C ₇ H ₅ NOS		+	
Benzothiazole	C ₇ H ₅ NS	+		
Methyl 2-pyridyl ketone	C ₇ H ₇ NO	+		
Methyl 3-pyridyl ketone	C ₇ H ₇ NO	+		
Methyl nicotinate	C ₇ H ₇ NO ₂	+		
2-Methyl-6-vinylpyrazine	C ₇ H ₈ N ₂			+
6,7-Dihydro-5 <i>H</i> -cyclopentapyrazine	C ₇ H ₈ N ₂	+		
2,5-Lutidine	C ₇ H ₉ N			+
2,6-Lutidine	C ₇ H ₉ N		+	+
3,5-Lutidine	C ₇ H ₉ N			+
2-Ethylpyridine	C ₇ H ₉ N			+
4-Ethylpyridine	C ₇ H ₉ N			+
1-Ethylpyrrole-2-carboxaldehyde	C ₇ H ₉ NO			+
Methyl 5-methyl-2-pyrrolyl ketone	C ₇ H ₉ NO	+		
Trimethylpyrazine	C ₇ H ₁₀ N ₂	+		+
3-Ethyl-2-methylpyrazine	C ₇ H ₁₀ N ₂	+		+
5-Ethyl-2-methylpyrazine	C ₇ H ₁₀ N ₂	+		+

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
6-Ethyl-2-methylpyrazine	$C_7H_{10}N_2$	+		+
5-Oxoproline ethyl ester	$C_7H_{11}NO_3$		+	
2-Furylpyrazine	$C_8H_6N_2O$	+		
Indone	C_8H_7N	+	+	
5-Methylcyclopentapyrazine	$C_8H_8N_2$	+		
Ethyl nicotinate	$C_8H_9NO_2$	+		
6,7-Dihydro-2-methyl-5 <i>H</i> -cyclopentapyrazine	$C_8H_{10}N_2$	+		
6,7-Dihydro-5-methyl-5 <i>H</i> -cyclopentapyrazine	$C_8H_{10}N_2$	+		
5-Ethyl-2-methylpyridine	$C_8H_{11}N$			+
2-Isopropylpyridine	$C_8H_{11}N$			+
Tetramethylpyrazine	$C_8H_{12}N_2$	+		+
3,5-Dimethyl-2-ethylpyrazine	$C_8H_{12}N_2$	+		+
2,5-Dimethyl-3-ethylpyrazine	$C_8H_{12}N_2$	+		+
5,6-Dimethyl-2-ethylpyrazine	$C_8H_{12}N_2$	+		
2,5-Diethylpyrazine	$C_8H_{12}N_2$			+
Quinoline	C_9H_7N			+
2-(2'-Furyl)methylpyrazine	$C_9H_8N_2O$	+		
1-Furfurylpyrrole	C_9H_9NO	+		
2,4-Dimethyl-3-propylpyrazine	$C_9H_{14}N_2$			+
Quinaldine	$C_{10}H_9N$			+
6-Methylquinoline	$C_{10}H_9N$			+
<i>N</i> -Furfurylpyrrol-2-aldehyde	$C_{10}H_9NO_2$	+		
3-Indolylacetic acid	$C_{10}H_9NO_2$		+	
5-Methoxy-2-indolylcarboxylic acid	$C_{10}H_9NO_3$		+	
2-(2'-Furyl)dimethylpyrazine	$C_{10}H_{10}N_2O$	+		
Ethylindole	$C_{10}H_{11}N$		+	
Indole-3-ethanol	$C_{10}H_{11}NO$	+	+	
3-(2-Aminoethyl)indole	$C_{10}H_{12}N_2$	+		
3-(2-Aminoethyl)indol-5-ol	$C_{10}H_{12}N_2O$	+		
1-Isopentylpyrrole-2-carboxaldehyde	$C_{10}H_{15}NO$			+
3-(3-Indolyl)propenoic acid	$C_{11}H_9NO_2$		+	
Isopentyl nicotinate	$C_{11}H_{15}NO_2$	+		
Phenethyl nicotinate	$C_{14}H_{13}NO_2$	+		
<i>Sulphur compounds</i>				
Thioformaldehyde	CH_2S	+		
Methanethiol	CH_4S	+		+
Carbon disulphide	CS_2		+	+
Dithioformaldehyde	$C_2H_4S_2$	+		
Ethanethiol	C_2H_6S	+	+	+
Methyl sulphide	C_2H_6S	+	+	+
Methyl disulphide	$C_2H_6S_2$	+	+	+
Dimethyl trisulphide	$C_2H_6S_3$	+	+	+
Thiazole	C_3H_3NS	+		+
<i>S</i> -Methyl thioacetate	C_3H_6OS	+	+	

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
(Methylthio)acetic acid	$C_3H_6O_2S$	+		
2-Propanethione	C_3H_6S	+		
2-Propene-1-thiol	C_3H_6S	+		
Ethyl methyl sulphide	C_3H_8S	+		
Ethyl methyl disulphide	$C_3H_8S_2$	+		
3-(Methylthio)propionaldehyde	C_3H_8OS	+		
S-Ethyl thioacetate	C_4H_8OS	+	+	
3-(Methylthio)propionic acid	$C_4H_8O_2S$	+	+	
Tetrahydrothiophene	C_4H_8S		+	
3-(Methylthio)-1-propanol	$C_4H_{10}OS$	+	+	+
Diethyl sulphite	$C_4H_{10}O_3S$			+
2-Methyl-2-propanethiol	$C_4H_{10}S$	+		
2-Methyl-2-propanethiol	$C_4H_{10}S$	+		
Ethyl sulphide	$C_4H_{10}S$	+		+
Ethyl disulphide	$C_4H_{10}S_2$	+		+
2-Thiophenecarboxaldehyde	C_5H_4OS	+		+
2-Thiophenecarboxylic acid	$C_5H_4O_2S$	+		
Dihydro-2-methyl-3(2 <i>H</i>)-thiophenone	C_5H_8OS	+	+	
Methyl 3-(methylthio)propionate	$C_5H_{10}O_2S$		+	
3-Methyl-2-butene-1-thiol	$C_5H_{10}S$	+		
3-(Ethylthio)-1-propanol	$C_5H_{12}OS$		+	
1-Pentanethiol	$C_5H_{12}S$	+		
Butyl methyl sulphide	$C_5H_{12}S$	+		
Ethyl propyl sulphide	$C_5H_{12}S$	+		
1-(2-Thienyl)ethanone	C_6H_6OS	+		
2-Methyl-2-thiophenecarboxaldehyde	C_6H_6OS	+		+
Allyl sulphide	$C_6H_{10}S$			+
<i>N,S</i> -Diacetyl-2-aminoethanethiol	$C_6H_{11}NO_2S$		+	
3-(Methylthio)propyl acetate	$C_6H_{12}O_2S$	+	+	+
Ethyl 3-(methylthio)propionate	$C_6H_{12}O_2S$	+	+	+
<i>N</i> -[3-(Methylthio)propyl]acetamide	$C_6H_{13}NOS$		+	
Butyl ethyl sulphide	$C_6H_{14}S$	+		+
Isopropyl sulphide	$C_6H_{14}S$	+		+
Isopropyl disulphide	$C_6H_{14}S_2$			+
2-Benzothiazolol	C_7H_5NOS		+	
Benzothiazole	C_7H_5NS	+		
Ethyl 2-thiophenecarboxylate	$C_7H_8O_2S$			+
<i>S</i> -Methyl 4-methylpentanethioate	$C_7H_{14}OS$	+		
5-Methyl hexanethioate	$C_7H_{14}OS$	+		
2-(Methylthio)benzothiazole	$C_8H_7NS_2$			+
<i>tert</i> -Butyl sulphide	$C_8H_{18}S$	+		
Isobutyl sulphide	$C_8H_{18}S$	+		
4-(4-Methyl-3-pentenyl)-3,6-dihydro-1,2-dithiin	$C_{10}H_{16}S_2$	+		
Isopentyl sulphide	$C_{10}H_{22}S$			+
Hydrogen sulphide	H_2S	+	+	+

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
<i>Terpenoids</i>				
7,7-Dimethyl-6,8-dioxabicyclo[3.2.1]octane	C ₈ H ₁₄ O ₂	+		
<i>para</i> -Cymene	C ₁₀ H ₁₄		+	+
<i>para</i> -Isopropylbenzyl alcohol (Cuminy alcohol)	C ₁₀ H ₁₄ O			+
<i>meta</i> -Cymenol	C ₁₀ H ₁₄ O			+
<i>para</i> -Cymenol	C ₁₀ H ₁₄ O			+
<i>para</i> -Mentha-6,8-dien-2-one (<i>d</i> -Carvone)	C ₁₀ H ₁₄ O	+		+
2(10)-Pinen-3-one (Pinocarvone)	C ₁₀ H ₁₄ O			+
1,7,7-Trimethyltricyclo[2.2.1.0 ²⁶]heptane (Tricyclene)	C ₁₀ H ₁₆			+
7-Methyl-3-methylene-1,6-octadiene (Myrcene)	C ₁₀ H ₁₆	+	+	+
<i>para</i> -Mentha-1(7),2-diene (β -Phellandrene)	C ₁₀ H ₁₆			+
<i>para</i> -Mentha-1,3-diene (α -Terpinene)	C ₁₀ H ₁₆			+
<i>para</i> -Mentha-1,4-diene (γ -Terpinene)	C ₁₀ H ₁₆			+
<i>para</i> -Mentha-1,4(8)-diene (Terpinolene)	C ₁₀ H ₁₆			+
<i>para</i> -Mentha-1,5-diene (α -Phellandrene)	C ₁₀ H ₁₆			+
<i>para</i> -Mentha-1,8-diene (Limonene)	C ₁₀ H ₁₆	+	+	+
3-Thujene (α -Thujene)	C ₁₀ H ₁₆			+
4(10)-Thujene (Sabinene)	C ₁₀ H ₁₆			+
2-Pinene (α -Pinene)	C ₁₀ H ₁₆	+		+
2(10)-Pinene (β -Pinene)	C ₁₀ H ₁₆			+
Camphene	C ₁₀ H ₁₆			+
3-Carene	C ₁₀ H ₁₆			+
3,7-Dimethyl-1,5,7-octatrien-3-ol (Ho-trienol)	C ₁₀ H ₁₆ O		+	+
3,7-Dimethyl-2,6-octadienal (Citral)	C ₁₀ H ₁₆ O	+	+	
2-Methyl-6-methylene-7-octen-2-ol (Myrcenol)	C ₁₀ H ₁₆ O			+
2,6,6-Trimethyl-1-cyclohexene-1-carboxaldehyde (β -Cyclocitral)	C ₁₀ H ₁₆ O			+
4-Isopropyl-1-cyclohexene-1-carboxaldehyde (Phellandral)	C ₁₀ H ₁₆ O			+
8,8-Dimethyl-2-methylene-6-oxabicyclo-[3.2.1]octane (Karahana ether)	C ₁₀ H ₁₆ O	+		
Hexahydro-1,1-dimethyl-4-methylene-1 <i>H</i> -cyclopenta[<i>c</i>]furan (Hop ether)	C ₁₀ H ₁₆ O	+		
Tetrahydro-5-isopropenyl-2-methyl-2-vinylfuran	C ₁₀ H ₁₆ O			+
3,6-Dihydro-4-methyl-2-(2-methyl-1-propenyl)-2 <i>H</i> -pyran (Nerol oxide)	C ₁₀ H ₁₆ O		+	+
<i>para</i> -Mentha-1(7),8-dien-2-ol, <i>trans</i> -	C ₁₀ H ₁₆ O			+
<i>para</i> -Menth-3-en-2-one (Carvenone)	C ₁₀ H ₁₆ O			+
6,8-Epoxy- <i>para</i> -menth-1-ene (Pinol)	C ₁₀ H ₁₆ O			+
2(10)-Pinen-3-ol, <i>trans</i> - (<i>trans</i> -Pinocarveol)	C ₁₀ H ₁₆ O			+
2-Pinen-10-ol (Myrtenol)	C ₁₀ H ₁₆ O			+
1,3,3-Trimethyl-2-norbornanone (Fenchone)	C ₁₀ H ₁₆ O			+
2-Bornanone (Camphor)	C ₁₀ H ₁₆ O			+
3,7-Dimethyl-1,6-octadien-3-ol (Linalool)	C ₁₀ H ₁₈ O	+	+	+

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
Geraniol	$C_{10}H_{18}O$			
Geraniol, <i>cis</i> - (Nerol)		+	+	+
Geraniol, <i>trans</i> - (Geraniol)		+	+	+
Tetrahydro-4-methyl-2-(2-methyl-1-propenyl)-2H-pyran (Rose oxide)	$C_{10}H_{18}O$			
Rose oxide, <i>cis</i> -			+	+
Rose oxide, <i>trans</i> -			+	+
Terpineol	$C_{10}H_{18}O$	+		+
<i>para</i> -Menth-3-en-1-ol (3-Terpinen-1-ol)	$C_{10}H_{18}O$			+
<i>para</i> -Menth-4(8)-en-1-ol (γ -Terpineol)	$C_{10}H_{18}O$			+
<i>para</i> -Menth-8-en-1-ol, <i>trans</i> - (β -Terpineol)	$C_{10}H_{18}O$			+
<i>para</i> -Menth-6-en-2-ol, (2 <i>S</i> ,4 <i>S</i>)-(P)-(<i>cis</i> -Carvotanacetol)	$C_{10}H_{18}O$			+
<i>para</i> -Menth-8-en-3-ol, (1 <i>R</i> ,3 <i>R</i> ,4 <i>S</i>)-(M)- (Isopulegol)	$C_{10}H_{18}O$			+
<i>para</i> -Menth-1-en-4-ol (4-Terpineol)	$C_{10}H_{18}O$	+	+	+
<i>para</i> -Menth-1-en-8-ol (α -Terpineol)	$C_{10}H_{18}O$	+	+	+
<i>para</i> -Menth-1-en-9-ol	$C_{10}H_{18}O$			+
<i>para</i> -Menth-2-one, <i>trans</i> - (Carvomenthone)	$C_{10}H_{18}O$			+
1,4-Epoxy- <i>para</i> -menthane (1,4-Cineole)	$C_{10}H_{18}O$			+
1,8-Epoxy- <i>para</i> -menthane (1,8-Cineole)	$C_{10}H_{18}O$	+		+
Isoborneol (<i>exo</i> -2-Bornanol)	$C_{10}H_{18}O$			+
Borneol (<i>endo</i> -2-Bornanol)	$C_{10}H_{18}O$			+
1,3,3-Trimethyl-2-norbornanol (Fenchol)	$C_{10}H_{18}O$	+		
1,3,3-Trimethyl-2-norbornanol, <i>endo</i> - (α -Fenchol)	$C_{10}H_{18}O$			+
3,7-Dimethylocta-1,5-dien-3,7-diol	$C_{10}H_{18}O_2$		+	
Tetrahydro- $\alpha,\alpha,5$ -trimethyl-5-vinyl-furfuryl alcohol (Linalool oxide)	$C_{10}H_{18}O_2$			
Linalool oxide, <i>cis</i> -			+	+
Linalool oxide, <i>trans</i> -		+	+	+
Linalool oxide, crystalline			+	
3,7-Dimethyl-6-octen-1-ol (Citronellol)	$C_{10}H_{20}O$	+		+
Menthol	$C_{10}H_{20}O$			+
3-Methyl-2-(2-pentenyl)-2-cyclopenten-1-one, <i>cis</i> - (Jasmone)	$C_{11}H_{16}O$	+		
2,2,7,7-Tetramethyl-1,6-dioxaspiro[4,4]-nona-3,8-diene	$C_{11}H_{16}O_2$	+		
2,2,7,7-Tetramethyl-1,6-dioxaspiro[4,4]-non-3-ene	$C_{11}H_{18}O_2$	+		
Linalyl acetate	$C_{12}H_{20}O_2$			+
Geranyl acetate	$C_{12}H_{20}O_2$			+
Bornyl acetate	$C_{12}H_{20}O_2$			+
Ethyl geranyl ether	$C_{12}H_{22}O$			+

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
1-(6,6-Dimethyl-2-methylene-3-cyclohexen-yl)-1-buten-3-one, <i>trans</i> -	C ₁₃ H ₁₈ O			+
1-(2,6,6-Trimethyl-1,3-cyclohexadien-1-yl)-2-buten-1-one (Damascenone)	C ₁₃ H ₁₈ O	+	+	+
Damascenone, <i>cis</i> -				+
Damascenone, <i>trans</i> -				+
Ionone	C ₁₃ H ₂₀ O			+
4-(2,6,6-Trimethyl-2-cyclohexen-1-yl)-3-buten-2-one, <i>trans</i> - (α -Ionone)	C ₁₃ H ₂₀ O	+	+	+
4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-3-buten-2-one (β -Ionone)	C ₁₃ H ₂₀ O	+	+	+
3,5,6,8a-Tetrahydro-2,5,5,8a-tetramethyl-2H-1-benzopyran, <i>trans</i> - (<i>trans</i> -Edulan; Edulan I)	C ₁₃ H ₂₀ O			+
3,4,4a,5,6,8a-Hexahydro-2,5,5,8-tetramethyl-4,4a-epoxy-2H-1-benzopyran (4,4a-Epoxyedulan)	C ₁₃ H ₂₀ O			+
Geranylacetone	C ₁₃ H ₂₂ O			+
5-(1-Hydroxy-2,6,6-trimethyl-4-oxo-2-cyclohexen-1-yl)-3-methyl-2,4-pentadienoic acid (Absciscic acid)	C ₁₅ H ₂₀ O ₄		+	
3,7,11-Trimethyl-1,3,6,10-dodecatetraene (Farnesene; α -Farnesene)	C ₁₅ H ₂₄	+		+
7,11-Dimethyl-3-methylene-1,8,10-dodecatriene (β -Farnesene)	C ₁₅ H ₂₄			+
2,6,6,9-Tetramethyl-1,4,8-cycloundecatriene <i>trans,trans,trans</i> - (Humulene; α -Caryophyllene)	C ₁₅ H ₂₄	+		+
4,11,11-Trimethyl-8-methylenebicyclo[7.2.0]-undec-4-ene,	C ₁₅ H ₂₄			
<i>cis</i> -(1 <i>R</i> ,9 <i>S</i>)-(M)- (Isocaryophyllene)		+		
<i>trans</i> -(1 <i>R</i> ,9 <i>S</i>)-(M)- (Caryophyllene; β -Caryophyllene)		+		+
1,3-Dimethyl-8-isopropyltricyclo-[4.4.0.0 ^{2,7}]dec-3-ene (α -Copaene)	C ₁₅ H ₂₄			+
1,2,3,5,6,8a-Hexahydro-4,7-dimethyl-1-isopropyl-naphthalene (δ -Cadinene)	C ₁₅ H ₂₄			+
1,2,4a,5,6,8a-Hexahydro-4,7-dimethyl-1-isopropyl-naphthalene, (1 <i>S</i>)-(1,4 <i>a</i> ,8 <i>a</i>)-(α -Muurolene)	C ₁₅ H ₂₄			+
1,2,3,4,4a,5,6,8a-Octahydro-7-methyl-4-methylene-1-isopropyl-naphthalene,	C ₁₅ H ₂₄			
(1 <i>a</i> ,4 <i>a</i> ,8 <i>a</i>)-(γ -Muurolene),				+
(1 <i>a</i> ,4 <i>a</i> ,8 <i>a</i>)-(γ -Cadinene)				+
3a,3b,4,5,6,7-Hexahydro-4-isopropyl-3,7-dimethyl-1H-cyclopenta(1,3)cyclopropana(1,2)benzene, (3 <i>a</i> ,3 <i>b</i> ,4 <i>a</i> ,7 <i>b</i>)-(M)- (α -Cubebene)	C ₁₅ H ₂₄			+
3,3,7-Trimethyl-11-methylene-4,7-cycloundecadien-1-ol, <i>trans,trans</i> -(<i>R</i>)-(P)- (Humulenol I)	C ₁₅ H ₂₄ O	+		

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
6,6,9-Trimethyl-2-methylene-4,8-cycloundecadien-1-ol, <i>trans,trans</i> -(<i>R</i>)-(<i>P</i>)- (Humulenol; Humulenol II)	C ₁₅ H ₂₄ O	+		
2,6,6,9-Tetramethyl-4,8-cycloundecadien-1-one, <i>trans,trans</i> -(<i>P</i>)- (Humuladienone)	C ₁₅ H ₂₄ O	+		
4,11,11-Trimethyl-8-methylenebicyclo[7.2.0]undec-3-en-5-ol (Caryophyllenol)	C ₁₅ H ₂₄ O	+		
1,5,5,8-Tetramethyl-12-oxabicyclo[9.1.0]-dodeca-3,7-diene, <i>trans,trans</i> -(1 <i>R</i> ,11 <i>R</i>)-(<i>M</i>)- (Humulene epoxide II)	C ₁₅ H ₂₄ O	+		
1,5,9,9-Tetramethyl-12-oxabicyclo[9.1.0]-dodeca-4,7-diene, <i>trans,trans</i> -(1 <i>R</i> ,11 <i>R</i>)-(<i>M</i>)- (Humulene epoxide; Humulene epoxide I)	C ₁₅ H ₂₄ O	+		
1,3-Dimethyl-3,4-epoxy-8-isopropyltricyclo[4.4.0.0 ^{2,7}]decane (α -Copaene epoxide)	C ₁₅ H ₂₄ O			+
4,12,12-Trimethyl-9-methylene-5-oxatricyclo[8.2.0.0 ^{4,6}]dodecane, (1 <i>R</i> ,4 <i>R</i> ,6 <i>R</i> ,10 <i>S</i>)- (Caryophyllene epoxide)	C ₁₅ H ₂₄ O	+		
1-(2,6,6-Trimethyl-1,3-cyclohexadien-1-yl)-3-ethoxybutan-1-one	C ₁₅ H ₂₄ O ₂			+
3,7,11-Trimethyl-1,6,10-dodecatrien-3-ol (Nerolidol)	C ₁₅ H ₂₆ O	+		+
3,7,11-Trimethyl-2,6,10-dodecatrien-1-ol (Farnesol)	C ₁₅ H ₂₆ O		+	
Farnesol, <i>cis</i> -			+	
Farnesol, <i>trans</i> -			+	
1,5,5,8-Tetramethyl-3,7-cycloundecadien-1-ol, <i>trans,trans</i> -(<i>M</i>)- (Humulol)	C ₁₅ H ₂₆ O	+		
4,4,8-Trimethyltricyclo[6.3.1.0 ^{2,5}]dodecan-1-ol- (Caryolan-1-ol)	C ₁₅ H ₂₆ O	+		
1,3,4,5,6,8a-Hexahydro-4,7-dimethyl-1-isopropyl-4a(2 <i>H</i>)-naphthalenol, (1 <i>S</i>)- (1 α ,4 β ,4 α ,8 α)- (Epicubenol)	C ₁₅ H ₂₆ O	+		
Cadinol	C ₁₅ H ₂₆ O	+		
1,2,3,4,4a,7,8,8a-Octahydro-1,6-dimethyl-4-isopropyl-1-naphthalenol	C ₁₅ H ₂₆ O			
, (1 <i>R</i>)-(1 α ,4 β ,4 α ,8 α)- (α -Cadinol)				+
, (1 <i>S</i>)-(1 α ,4 α ,4 α ,8 α)- (δ -Cadinol)		+		+
, (1 <i>S</i>)-(1 α ,4 α ,4 α ,8 α)- (τ -Cadinol)		+		
Decahydro-4a-methyl-8-methylene-2-isopropyl-1-naphthalenol, (1 <i>S</i>)-(1 α ,2 β ,4 α ,8 α)- (Junenol)	C ₁₅ H ₂₆ O	+		
<i>Phenols and phenyl ethers</i>				
Phenol	C ₆ H ₆ O	+	+	+

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
Pyrocatechol	C ₆ H ₆ O ₂	+	+	
Resorcinol (IARC, 1977b, 1987a)	C ₆ H ₆ O ₂	+	+	
Pyrogallol	C ₆ H ₆ O ₃	+	+	
Phloroglucinol	C ₆ H ₆ O ₃	+	+	
Cresol	C ₇ H ₈ O	+		
<i>ortho</i> -Cresol	C ₇ H ₈ O	+	+	+
<i>meta</i> -Cresol	C ₇ H ₈ O	+	+	+
<i>para</i> -Cresol	C ₇ H ₈ O	+	+	+
5-Methylresorcinol	C ₇ H ₈ O ₂	+	+	
<i>ortho</i> -Methoxyphenol	C ₇ H ₈ O ₂	+	+	+
<i>para</i> -Vinylphenol	C ₈ H ₈ O	+	+	+
2,5-Xylenol	C ₈ H ₁₀ O			+
2,6-Xylenol	C ₈ H ₁₀ O			+
3,5-Xylenol	C ₈ H ₁₀ O			+
Ethylphenol	C ₈ H ₁₀ O			+
<i>ortho</i> -Ethylphenol	C ₈ H ₁₀ O		+	+
<i>meta</i> -Ethylphenol	C ₈ H ₁₀ O			+
<i>para</i> -Ethylphenol	C ₈ H ₁₀ O	+	+	+
<i>ortho</i> -Dimethoxybenzene	C ₈ H ₁₀ O ₂	+		+
<i>meta</i> -Dimethoxybenzene	C ₈ H ₁₀ O ₂			+
2-Methoxy-4-methylphenol	C ₈ H ₁₀ O ₂	+	+	+
2-Methoxy-6-methylphenol	C ₈ H ₁₀ O ₂			+
4-Ethylpyrocatechol	C ₈ H ₁₀ O ₂		+	
2,6-Dimethoxyphenol	C ₈ H ₁₀ O ₃	+	+	+
Vanillyl alcohol	C ₈ H ₁₀ O ₃	+		
<i>para</i> -Allylphenol	C ₉ H ₁₀ O		+	
<i>para</i> -Propenylphenol	C ₉ H ₁₀ O		+	
Vinyl-2-methoxyphenol	C ₉ H ₁₀ O ₂	+		
4-Vinyl-2-methoxyphenol	C ₉ H ₁₀ O ₂	+	+	+
2,3,5-Trimethylphenol	C ₉ H ₁₂ O			+
2,4,5-Trimethylphenol	C ₉ H ₁₂ O			+
Mesitol	C ₉ H ₁₂ O			+
<i>ortho</i> -Isopropylphenol	C ₉ H ₁₂ O			+
<i>para</i> -Propylphenol	C ₉ H ₁₂ O	+		
Ethyl-2-methoxyphenol	C ₉ H ₁₂ O ₂			+
4-Ethyl-2-methoxyphenol	C ₉ H ₁₂ O ₂	+	+	+
2,6-Dimethoxy-4-methylphenol	C ₉ H ₁₂ O ₃	+		
Trimethoxyphenol	C ₉ H ₁₂ O ₄		+	
1-Naphthol	C ₁₀ H ₈ O		+	
1-Allyl-methoxybenzene	C ₁₀ H ₁₂ O		+	
2-Methoxy-4-propenylphenol	C ₁₀ H ₁₂ O ₂	+	+	+
4-Allyl-2-methoxyphenol (Eugenol) (IARC, 1985, 1987a)	C ₁₀ H ₁₂ O ₂	+	+	+

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
3-(4-Hydroxy-3-methoxyphenyl)-2-propen-1-ol	C ₁₀ H ₁₂ O ₃			+
4-Vinyl-2,6-dimethoxyphenol	C ₁₀ H ₁₂ O ₃	+		+
Tetramethylphenol	C ₁₀ H ₁₄ O			+
Carvacrol	C ₁₀ H ₁₄ O	+		+
Thymol	C ₁₀ H ₁₄ O			+
Propyl-2-methoxyphenol	C ₁₀ H ₁₄ O ₂			+
2-Methoxy-4-propylphenol	C ₁₀ H ₁₄ O ₂			+
1-Ethoxy-1-(4-methoxyphenyl)ethane	C ₁₀ H ₁₄ O ₂			+
Ethyl 4-methoxybenzyl ether	C ₁₀ H ₁₄ O ₂			+
4-Ethyl-2,6-dimethoxyphenol	C ₁₀ H ₁₄ O ₃	+	+	+
Ethyl vanillyl ether	C ₁₀ H ₁₄ O ₃			+
4-Allyl-1,2-dimethoxybenzene	C ₁₁ H ₁₄ O ₂		+	
Methyl-4-allyl-2-methoxyphenol	C ₁₁ H ₁₄ O ₂			+
4-Propenyl-2,6-dimethoxyphenol	C ₁₁ H ₁₄ O ₃	+		
4-Allyl-2,6-dimethoxyphenol	C ₁₁ H ₁₄ O ₃	+		
Isopropyl-2,6-dimethoxyphenol	C ₁₁ H ₁₆ O ₃		+	
2,6-Di- <i>tert</i> -butyl-4-methylphenol	C ₁₅ H ₂₄ O		+	
<i>Aromatic alcohols</i>				
Benzyl alcohol	C ₇ H ₈ O	+	+	+
1-Phenylethyl alcohol	C ₈ H ₁₀ O		+	+
Phenethyl alcohol	C ₈ H ₁₀ O	+	+	+
Tyrosol	C ₈ H ₁₀ O ₂	+	+	
Cinnamyl alcohol	C ₉ H ₁₀ O			+
3-Phenylpropanol	C ₉ H ₁₂ O		+	
Methoxytyrosol	C ₉ H ₁₂ O ₃		+	
<i>Aromatic aldehydes and ketones</i>				
Benzaldehyde	C ₇ H ₆ O	+	+	+
Salicylaldehyde	C ₇ H ₆ O ₂	+	+	+
<i>para</i> -Hydroxybenzaldehyde	C ₇ H ₆ O ₂	+	+	+
Protocatechualdehyde	C ₇ H ₆ O ₃	+	+	+
Piperonal	C ₈ H ₆ O ₃	+	+	
<i>ortho</i> -Tolualdehyde	C ₈ H ₈ O			+
<i>meta</i> -Tolualdehyde	C ₈ H ₈ O			+
<i>para</i> -Tolualdehyde	C ₈ H ₈ O	+		
Phenylacetaldehyde	C ₈ H ₈ O	+	+	+
Acetophenone	C ₈ H ₈ O		+	+
Hydroxymethylbenzaldehyde	C ₈ H ₈ O ₂			+
<i>para</i> -Anisaldehyde	C ₈ H ₈ O ₂	+		+
2'-Hydroxyacetophenone	C ₈ H ₈ O ₂		+	
4'-Hydroxyacetophenone	C ₈ H ₈ O ₂	+	+	
Vanillin	C ₈ H ₈ O ₃	+	+	+
Cinnamaldehyde	C ₉ H ₈ O	+	+	+
1-Indanone	C ₉ H ₈ O	+		+
2,4-Dimethylbenzaldehyde	C ₉ H ₁₀ O			+

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
Ethylbenzaldehyde	C ₉ H ₁₀ O		+	
4-Ethylbenzaldehyde	C ₉ H ₁₀ O		+	
Hydrocinnamaldehyde	C ₉ H ₁₀ O	+		
3-Phenyl-2-propanone	C ₉ H ₁₀ O			+
4'-Methylacetophenone	C ₉ H ₁₀ O			+
2'-Hydroxy-5'-methylacetophenone	C ₉ H ₁₀ O ₂			+
2-Ethoxybenzaldehyde	C ₉ H ₁₀ O ₂			+
4'-Hydroxy-3'-methoxyacetophenone	C ₉ H ₁₀ O ₃	+	+	+
4-Hydroxy-3,5-dimethoxybenzaldehyde	C ₉ H ₁₀ O ₄	+	+	+
4-Hydroxy-3-methoxycinnamaldehyde	C ₁₀ H ₁₀ O ₃			+
Ethylacetophenone	C ₁₀ H ₁₂ O		+	
4'-Ethylacetophenone	C ₁₀ H ₁₂ O		+	
<i>para</i> -Isopropylbenzaldehyde	C ₁₀ H ₁₂ O			+
3-Hydroxy-4-phenyl-2-butanone	C ₁₀ H ₁₂ O ₂		+	
4-Acetyl-2-methoxyphenol	C ₁₀ H ₁₂ O ₃	+		
4'-Hydroxy-3'-methoxypropiofenone	C ₁₀ H ₁₂ O ₃			+
4'-Hydroxy-3',5'-dimethoxyacetophenone	C ₁₀ H ₁₂ O ₄	+	+	+
4-Hydroxy-3,5-dimethoxycinnamaldehyde	C ₁₁ H ₁₂ O ₄			+
4-Acetyl-2,6-dimethoxyphenol	C ₁₁ H ₁₄ O ₄	+		
4'-Hydroxy-3',5'-dimethoxypropiofenone	C ₁₁ H ₁₄ O ₄			+
2'-Methyl-5'-isopropylacetophenone	C ₁₂ H ₁₆ O			+
1-(2,3,6-Trimethylphenyl)-2-buten-1-one	C ₁₃ H ₁₆ O			
, <i>cis</i> -				+
, <i>trans</i> -				+
4-(2,3,6-Trimethylphenyl)-3-buten-2-one	C ₁₃ H ₁₆ O			+
<i>Aromatic and other carboxylic acids</i>				
Benzoic acid	C ₇ H ₆ O ₂	+	+	+
Salicylic acid	C ₇ H ₆ O ₂	+	+	+
<i>para</i> -Hydroxybenzoic acid	C ₇ H ₆ O ₃	+	+	+
<i>ortho</i> -Pyrocatechuic acid	C ₇ H ₆ O ₄	+	+	
α -Resorcylic acid	C ₇ H ₆ O ₄	+	+	
β -Resorcylic acid	C ₇ H ₆ O ₄	+	+	
γ -Resorcylic acid	C ₇ H ₆ O ₄	+	+	
Gentisic acid	C ₇ H ₆ O ₄	+	+	+
Protocatechuic acid	C ₇ H ₆ O ₄	+	+	+
Gallic acid	C ₇ H ₆ O ₅	+	+	+
2,4,6-Trihydroxybenzoic acid	C ₇ H ₆ O ₅		+	
3,4,5-Trihydroxy-1-cyclohexene-1-carboxylic acid	C ₇ H ₁₀ O ₅	+	+	
1,3,4,5-Tetrahydroxycyclohexanecarboxylic acid	C ₇ H ₁₂ O ₆	+	+	+
Phenylglyoxylic acid	C ₈ H ₆ O ₃	+		
Phthalic acid	C ₈ H ₆ O ₄	+	+	+
<i>para</i> -Toluic acid	C ₈ H ₈ O ₂		+	
Phenylacetic acid	C ₈ H ₈ O ₂	+	+	+
<i>para</i> -Hydroxyphenylacetic acid	C ₈ H ₈ O ₃	+	+	

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
Vanillic acid	$C_8H_8O_4$	+	+	+
Cinnamic acid	$C_9H_8O_3$	+	+	+
Cinnamic acid, <i>cis</i> -		+		
Cinnamic acid, <i>trans</i> -		+		
<i>ortho</i> -Hydroxycinnamic acid	$C_9H_8O_3$	+	+	
<i>meta</i> -Hydroxycinnamic acid	$C_9H_8O_3$	+	+	
<i>para</i> -Hydroxycinnamic acid	$C_9H_8O_3$	+	+	+
<i>para</i> -Hydroxycinnamic acid, <i>cis</i> -		+	+	
<i>para</i> -Hydroxycinnamic acid, <i>trans</i> -		+	+	
Phenylpyruvic acid	$C_9H_8O_3$	+	+	
3,4-Dihydroxycinnamic acid	$C_9H_8O_4$	+	+	+
3,4-Dihydroxycinnamic acid, <i>cis</i> -			+	
3,4-Dihydroxycinnamic acid, <i>trans</i> -			+	
<i>para</i> -Hydroxyphenylpyruvic acid	$C_9H_8O_4$		+	
Phenylpropionic acid	$C_9H_{10}O_2$	+	+	+
Hydratropic acid	$C_9H_{10}O_2$		+	
Hydrocinnamic acid	$C_9H_{10}O_2$	+	+	+
<i>para</i> -Hydroxyphenylpropionic acid	$C_9H_{10}O_3$	+	+	
Phenyllactic acid	$C_9H_{10}O_3$	+		
3-Phenyllactic acid	$C_9H_{10}O_3$		+	
Veratric acid	$C_9H_{10}O_4$	+	+	
4-Hydroxy-3-methoxyphenylacetic acid	$C_9H_{10}O_4$		+	
3,4-Dihydroxyhydrocinnamic acid	$C_9H_{10}O_4$		+	
4-Hydroxy-3,5-dimethoxybenzoic acid	$C_9H_{10}O_5$	+	+	+
4-Hydroxy-3-methoxycinnamic acid	$C_{10}H_{10}O_4$	+	+	+
4-Hydroxy-3-methoxycinnamic acid, <i>cis</i> -		+		
4-Hydroxy-3-methoxycinnamic acid, <i>trans</i> -		+		
<i>para</i> -Hydroxyphenylbutyric acid	$C_{10}H_{12}O_3$		+	
4-Hydroxy-3,5-dimethoxycinnamic acid	$C_{10}H_{12}O_5$	+	+	
Tartaric acid mono(4-hydroxycinnamate)	$C_{13}H_{12}O_8$		+	
, <i>cis</i> -			+	
, <i>trans</i> -			+	
Tartaric acid mono(3,4-dihydroxycinnamate)	$C_{13}H_{12}O_9$		+	
, <i>trans</i> -			+	
Tartaric acid mono(4-hydroxy-3-methoxycinnamate)	$C_{14}H_{14}O_9$		+	
1,3,4,5-Tetrahydroxycyclohexanecarboxylic acid mono[3-(<i>para</i> -hydroxycinnamate)]	$C_{16}H_{18}O_8$		+	
Chlorogenic acid	$C_{16}H_{18}O_9$	+	+	+
Isochlorogenic acid	$C_{16}H_{18}O_9$	+	+	
Neochlorogenic acid	$C_{16}H_{18}O_9$	+	+	
<i>Esters of aromatic acids</i>				
Methyl benzoate	$C_8H_8O_2$			+
Methyl salicylate	$C_8H_8O_3$			+

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
Methyl anthranilate	$C_8H_9NO_2$		+	
Ethyl benzoate	$C_9H_{10}O_2$	+	+	+
Methyl phenylacetate	$C_9H_{10}O_2$			+
Ethyl salicylate	$C_9H_{10}O_3$		+	+
Ethyl <i>para</i> -hydroxybenzoate	$C_9H_{10}O_3$		+	
Dimethyl phthalate	$C_{10}H_{10}O_4$		+	+
Ethyl hydrogen phthalate	$C_{10}H_{10}O_4$		+	
Ethyl phenylacetate	$C_{10}H_{12}O_2$	+	+	+
Ethyl vanillate	$C_{10}H_{12}O_4$		+	+
Ethyl cinnamate	$C_{11}H_{12}O_2$	+	+	+
Isobutyl benzoate	$C_{11}H_{14}O_2$	+	+	
Ethyl 2-phenylpropionate	$C_{11}H_{14}O_2$			+
Ethyl hydrocinnamate	$C_{11}H_{14}O_2$			+
Ethyl 3-phenyllactate	$C_{11}H_{14}O_3$		+	
Ethyl 4-hydroxy-3,5-dimethoxybenzoate	$C_{11}H_{14}O_5$		+	+
Ethyl 4-phenyl-3-butenolate	$C_{12}H_{14}O_2$		+	
Diethyl phthalate	$C_{12}H_{14}O_4$		+	+
Isopentyl benzoate	$C_{12}H_{16}O_2$	+		
Pentyl benzoate	$C_{12}H_{16}O_2$	+		
Isopentyl salicylate	$C_{12}H_{16}O_3$			+
Diisobutyl phthalate	$C_{16}H_{22}O_4$		+	
Dibutyl phthalate	$C_{16}H_{22}O_4$		+	+
<i>Lactones</i>				
Dihydro-2(3 <i>H</i>)-furanone (γ -Butyrolactone) (IARC, 1976b, 1987a)	$C_4H_6O_2$	+	+	+
Tetrahydro-5-oxo-2-furoic acid	$C_5H_6O_4$		+	
Dihydro-3-methyl-2(3 <i>H</i>)-furanone	$C_5H_8O_2$		+	
Dihydro-5-methyl-2(3 <i>H</i>)-furanone	$C_5H_8O_2$	+	+	
Tetrahydro-2 <i>H</i> -pyran-2-one	$C_5H_8O_2$	+		
5,5-Dimethyl-2(5 <i>H</i>)-furanone	$C_6H_8O_2$	+		
4-Acetyldihydro-2(3 <i>H</i>)-furanone	$C_6H_8O_3$		+	
4,5-Dimethyl-2,3-tetrahydrofuranone	$C_6H_8O_3$		+	+
6-Methyldihydro-2,5(3 <i>H</i>)-pyrandione	$C_6H_8O_3$		+	
Dihydro-5,5-dimethyl-2(3 <i>H</i>)-furanone	$C_6H_{10}O_2$	+		
Tetrahydro-5-methyl-2 <i>H</i> -pyran-2-one	$C_6H_{10}O_2$	+		
5-Ethyldihydro-2(3 <i>H</i>)-furanone	$C_6H_{10}O_2$	+	+	+
Dihydro-3-hydroxy-4,4-dimethyl-2(3 <i>H</i>)-furanone	$C_6H_{10}O_3$		+	
Dihydro-5-ethoxy-2(3 <i>H</i>)-furanone	$C_6H_{10}O_3$		+	
Dihydro-5-(1-hydroxyethyl)-2(3 <i>H</i>)-furanone	$C_6H_{10}O_3$		+	
Dihydro-5-methyl-5-vinyl-2(3 <i>H</i>)-furanone	$C_7H_{10}O_2$		+	
5-Carbethoxydihydro-2(3 <i>H</i>)-furanone	$C_7H_{10}O_4$		+	
Dihydro-5-propyl-2(3 <i>H</i>)-furanone	$C_7H_{12}O_2$	+		
Phthalide	$C_8H_6O_2$		+	
5-Butyldihydro-2(3 <i>H</i>)-furanone	$C_8H_{14}O_2$	+		+

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
Tetrahydro-6-propyl-2 <i>H</i> -pyran-2-one	C ₈ H ₁₄ O ₂			+
Coumarin (IARC, 1976b, 1987a)	C ₉ H ₆ O ₂		+	+
7-Hydroxycoumarin	C ₉ H ₆ O ₃	+	+	
7,8-Dihydroxycoumarin	C ₉ H ₆ O ₄	+	+	
5-Butyl-4-methyldihydro-2(3 <i>H</i>)-furanone	C ₉ H ₁₆ O ₂		+	+
, <i>cis</i> -			+	+
, <i>trans</i> -			+	+
Hydroxynonanoic acid lactone	C ₉ H ₁₆ O ₂	+		
Dihydro-5-pentyl-2(3 <i>H</i>)-furanone	C ₉ H ₁₆ O ₂	+	+	+
6-Butyltetrahydro-2 <i>H</i> -pyran-2-one	C ₉ H ₁₆ O ₂			+
6-Methylcoumarin	C ₁₀ H ₈ O ₂			+
7-Hydroxy-6-methoxycoumarin	C ₁₀ H ₈ O ₄	+	+	+
Dihydro-4-methyl-5-pentyl-2(3 <i>H</i>)-furanone	C ₁₀ H ₁₈ O ₂			+
5-Hexyldihydro-2(3 <i>H</i>)-furanone	C ₁₀ H ₁₈ O ₂	+	+	+
Tetrahydro-6-pentyl-2 <i>H</i> -pyran-2-one	C ₁₀ H ₁₈ O ₂		+	+
Tetrahydro-4,4,7a-trimethyl-2(4 <i>H</i>)-benzofuranone	C ₁₁ H ₁₆ O ₂	+		
5-Heptyldihydro-2(3 <i>H</i>)-furanone	C ₁₁ H ₂₀ O ₂			+
Dihydro-5-octyl-2(3 <i>H</i>)-furanone	C ₁₂ H ₂₂ O ₂	+		+
6-Heptyltetrahydro-2 <i>H</i> -pyran-2-one	C ₁₂ H ₂₂ O ₂			+
2,3,7,8-Tetrahydroxy[1]benzopyrano[5,4,3- <i>cde</i>]-[1]-benzopyran-5,10-dione (Ellagic acid)	C ₁₄ H ₆ O ₈	+	+	+
<i>O-Heterocyclics</i> (see also lactones and terpenoids)				
Dihydrofuran	C ₄ H ₆ O			+
2-Furaldehyde	C ₅ H ₄ O ₂	+	+	+
2-Furoic acid	C ₅ H ₄ O ₃	+	+	+
3-Furoic acid	C ₅ H ₄ O ₃			+
2-Methylfuran	C ₅ H ₆ O			+
Furfuryl alcohol	C ₅ H ₆ O ₂	+	+	+
Dihydro-2-methyl-3(2 <i>H</i>)-furanone	C ₅ H ₈ O ₂	+		+
2-Methyltetrahydrofuran	C ₅ H ₁₀ O			+
Furan-3,4-dicarboxylic acid	C ₆ H ₄ O ₅		+	
3-Methyl-2-furaldehyde	C ₆ H ₆ O ₂			+
5-Methyl-2-furaldehyde	C ₆ H ₆ O ₂	+	+	+
Furyl methyl ketone	C ₆ H ₆ O ₂	+		+
2-Furyl methyl ketone	C ₆ H ₆ O ₂	+		+
3-Furyl methyl ketone	C ₆ H ₆ O ₂			+
Methyl 2-furoate	C ₆ H ₆ O ₃			+
Hydroxymethyl-2-furaldehyde	C ₆ H ₆ O ₃	+	+	+
5-Hydroxymethyl-2-furaldehyde	C ₆ H ₆ O ₃	+		
2-Acetyl-3-hydroxyfuran	C ₆ H ₆ O ₃	+		
3-Hydroxy-2-methyl-4 <i>H</i> -pyran-4-one	C ₆ H ₆ O ₃	+		
5-Hydroxy-2-(hydroxymethyl)-4 <i>H</i> -pyran-4-one	C ₆ H ₆ O ₄	+		
3,5-Dihydroxy-2-methyl-4 <i>H</i> -pyran-4-one	C ₆ H ₆ O ₄	+		
5-Methylfurfuryl alcohol	C ₆ H ₈ O ₂	+		

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
5-Hydroxymethylfurfuryl alcohol	C ₆ H ₈ O ₃	+		
4-Hydroxy-2,5-dimethyl-3(2 <i>H</i>)-furanone	C ₆ H ₈ O ₃	+		
2,5-Di(hydroxymethyl)furan	C ₆ H ₈ O ₃	+		
3,5-Dihydroxy-2-methyl-5,6-dihydro-4 <i>H</i> -pyran-4-one	C ₆ H ₈ O ₄	+		
2,5-Dimethoxytetrahydrofuran	C ₆ H ₁₂ O ₃			+
5-Methyl-2-acetylfuran	C ₇ H ₈ O ₂	+		+
1-(2-Furyl)-1-propanone	C ₇ H ₈ O ₂	+		+
Ethyl furoate	C ₇ H ₈ O ₃		+	
Ethyl 2-furoate	C ₇ H ₈ O ₃	+	+	+
Ethyl furfuryl ether	C ₇ H ₁₀ O ₂		+	+
Propyl tetrahydrofuryl ether	C ₇ H ₁₄ O ₂		+	
1-(2-Furyl)-2-buten-1-one	C ₈ H ₈ O ₂			+
3-Acetyl-4-hydroxy-6-methyl-2 <i>H</i> -pyran-2-one	C ₈ H ₈ O ₄			+
Propyl furoate	C ₈ H ₁₀ O ₃		+	
2-Acetyl-4,5-dimethylfuran	C ₈ H ₁₀ O ₂			+
2-Acetyl-5-ethylfuran	C ₈ H ₁₀ O ₂			+
1-(2-Furyl)-1-penten-3-one	C ₉ H ₁₀ O ₂			+
Ethyl 3-(2-furyl)acrylate	C ₉ H ₁₀ O ₃			+
Isobutyl 2-furoate	C ₉ H ₁₂ O ₃			+
Butylfuryl alcohol	C ₉ H ₁₄ O ₂		+	
Isopentyl 2-furoate	C ₁₀ H ₁₄ O ₃			+
Tetrahydro-2,6,6-trimethyl-2-vinyl-4-hydroxypyran	C ₁₀ H ₁₈ O ₂		+	
Tetrahydro-2,6,6-trimethyl-2-vinyl-4-acetoxypyran	C ₁₂ H ₂₀ O ₃			
<i>Hydrocarbons (see also terpenoids)</i>				
Methane	CH ₄	+		
Propene	C ₃ H ₆	+		
Propane	C ₃ H ₈	+		
2-Methylpropene	C ₄ H ₈	+		
Isobutane	C ₄ H ₁₀			+
Isoprene	C ₅ H ₈	+		
2-Methyl-2-butene	C ₅ H ₁₀	+		
Methylcyclobutane	C ₅ H ₁₀		+	
Pentane	C ₅ H ₁₂		+	+
Benzene (IARC, 1982a, 1987a)	C ₆ H ₆		+	+
Methylcyclopentane	C ₆ H ₁₂		+	
Cyclohexane	C ₆ H ₁₂	+	+	
2,2-Dimethylbutane	C ₆ H ₁₄		+	
2,3-Dimethylbutane	C ₆ H ₁₄		+	
2-Methylpentane	C ₆ H ₁₄			+
3-Methylpentane	C ₆ H ₁₄		+	
Hexane	C ₆ H ₁₄		+	+
Toluene	C ₇ H ₈	+		+

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
3,4-Dimethyl-2-pentene	C ₇ H ₁₄	+		
Methylcyclohexane	C ₇ H ₁₄		+	+
2,3-Dimethylpentane	C ₇ H ₁₆			+
2,4-Dimethylpentane	C ₇ H ₁₆		+	
2-Methylhexane	C ₇ H ₁₆			+
Heptane	C ₇ H ₁₆		+	+
Styrene (IARC, 1979a, 1987a)	C ₈ H ₈	+	+	+
<i>ortho</i> -Xylene	C ₈ H ₁₀	+		
<i>meta</i> -Xylene	C ₈ H ₁₀		+	
Ethylbenzene	C ₈ H ₁₀	+		
2,2-Dimethylhexane	C ₈ H ₁₈	+		
Indene	C ₉ H ₈		+	
Methylethylbenzene	C ₉ H ₁₂	+		
Isopropyl benzene	C ₉ H ₁₂		+	
Propylbenzene	C ₉ H ₁₂		+	
Naphthalene	C ₁₀ H ₈	+	+	+
α -Dimethylstyrene	C ₁₀ H ₁₂			+
Isobutylbenzene	C ₁₀ H ₁₄	+		
Decane	C ₁₀ H ₂₂		+	
Methylnaphthalene	C ₁₁ H ₁₀			+
1,3-Dimethylnaphthalene	C ₁₂ H ₁₂			+
2,6-Dimethylnaphthalene	C ₁₂ H ₁₂			+
Dodecane	C ₁₂ H ₂₆		+	
Trimethyldihydronaphthalene	C ₁₃ H ₁₆		+	
1,1,6-Trimethyl-1,2-dihydronaphthalene	C ₁₃ H ₁₆		+	+
1-(2,3,6-Trimethylphenyl)-1,3-butadiene	C ₁₃ H ₁₆	+		+
1,1,6-Trimethyltetrahydronaphthalene	C ₁₃ H ₁₈		+	+
Anthracene (IARC, 1983c, 1987a)	C ₁₄ H ₁₀			+
Phenanthrene (IARC, 1983c, 1987a)	C ₁₄ H ₁₀			+
Tetradecane	C ₁₄ H ₃₀		+	
Pyrene (IARC, 1983c, 1987a)	C ₁₅ H ₁₀			+
Fluoranthene (IARC, 1983c, 1987a)	C ₁₆ H ₁₀			+
Hexadecane	C ₁₆ H ₃₄		+	
Benzo[<i>a</i>]fluorene (IARC, 1983c, 1987a)	C ₁₇ H ₁₂			+
Heptadecane	C ₁₇ H ₃₆		+	
Benz[<i>a</i>]anthracene (IARC, 1983c, 1987a)	C ₁₈ H ₁₂			+
Chrysene (IARC, 1983c, 1987a)	C ₁₈ H ₁₂			+
Octadecane	C ₁₈ H ₃₈		+	
Benzo[<i>a</i>]pyrene (IARC, 1983c, 1987a)	C ₂₀ H ₁₂			+
Benzo[<i>e</i>]pyrene (IARC, 1983c, 1987a)	C ₂₀ H ₁₂			+
Benzo[<i>b</i>]fluoranthene (IARC, 1983c, 1987a)	C ₂₀ H ₁₂			+
<i>Miscellaneous compounds</i>				
Chloroform (IARC, 1979b, 1987a)	CHCl ₃		+	
Bromoform	CHBr ₃			+

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
Trichloroethylene (IARC, 1979b, 1987a)	C ₂ HCl ₃		+	
1,1,2,3-Tetrachloro-3,3-difluoropropane	C ₃ H ₂ Cl ₄ F ₂		+	
Ethyl vinyl ether	C ₄ H ₈ O			+
Diethyl ether (IARC, 1976c, 1987a)	C ₄ H ₁₀ O	+	+	+
Diethyl carbonate	C ₅ H ₁₀ O ₃		+	+
Ethyl isopropyl ether	C ₅ H ₁₂ O		+	
Trichlorotrifluorobenzene	C ₆ Cl ₃ F ₃		+	
2,4,5,6-Tetrachloro-1,3-difluorobenzene	C ₆ Cl ₄ F ₂		+	
Dichlorobenzene (IARC, 1982a, 1987a)	C ₆ H ₄ Cl ₂			+
2,6-Dichlorophenol	C ₆ H ₄ OCl ₂			+
2-Chlorophenol	C ₆ H ₅ OCl			+
2,4,6-Trimethyl-1,3,5-trioxane	C ₆ H ₁₂ O ₃			+
Ethyl <i>tert</i> -butyl ether	C ₆ H ₁₄ O		+	
Ethyl <i>sec</i> -butyl ether	C ₆ H ₁₄ O		+	
Dibutyl ether	C ₈ H ₁₈ O			+
Bis(2-methylbutyl) carbonate	C ₁₁ H ₂₂ O ₃		+	
Diisopentyl carbonate	C ₁₁ H ₂₂ O ₃		+	
1,2,4-Trimethoxy-5-(1-propenyl)benzene, <i>cis</i> - (β -Asarone)	C ₁₂ H ₁₆ O ₃		+	
Octahydro-4,8a-dimethyl-4a(2 <i>H</i>)-naphthalenol (Geosmin)	C ₁₂ H ₂₀ O			+
2,6,6-Trimethyl-10-methylene-1-oxaspiro- [4.5]-8-decene (Vitispirane)	C ₁₃ H ₂₀ O		+	+
5,7,8,8a-Tetrahydro-2,5,5,8a-tetramethyl- 5 <i>H</i> -1-benzopyran	C ₁₃ H ₂₀ O			+
1-(2,3,6-Trimethylphenyl)-3-ethoxy-1-butene , <i>trans</i> -	C ₁₅ H ₂₂ O			+
Diphenethyl carbonate	C ₁₇ H ₁₈ O ₃		+	+

SOME OTHER COMPOUNDS

Aflatoxins (IARC, 1976b, 1987a)	C ₁₇ H ₁₂ O ₆	+	+	
Arsenic (IARC, 1980, 1987a)	As		+	
Asbestos (IARC, 1977a, 1987a)	—	+	+	+
Cadmium (IARC, 1976c, 1987a)	Cd		+	
Calcium	Ca	+	+	+
Chromium (IARC, 1980, 1987a)	Cr		+	
Cobalt	Co		+	
Copper	Cu	+	+	
Ethylene thiourea (IARC, 1974, 1987a)	C ₃ H ₆ N ₂ S		+	
Fluoride (IARC, 1982b, 1987a)	F		+	
Iron	Fe	+	+	
Lead (IARC, 1980, 1987a)	Pb		+	
Magnesium	Mg		+	+
Manganese	Mn		+	

Appendix 1 (contd)

Compound	Molecular formula	Identified in		
		Beer	Wine	Spirits
Nickel (IARC, 1976c, 1987a)	Ni		+	
Ochratoxin A (IARC, 1983a, 1987a)	C ₂₀ H ₁₈ ClNO ₆	+		
Phosphorus	P	+	+	
Potassium	K	+	+	+
Sodium	Na	+	+	+
Sulphur dioxide	SO ₂	+	+	
Sunset Yellow FCF (IARC, 1975, 1987a)	C ₁₆ H ₁₀ N ₂ Na ₂ O ₇ S ₂		+	+
Tannic acid and tannins (IARC, 1976b, 1987)	—		+	+
Trichlorfon (IARC, 1983b, 1987a)	C ₄ H ₈ Cl ₃ O ₄ P		+	
Zearalenone (IARC, 1983a, 1987a)	C ₁₈ H ₂₂ O ₅	+		
Zinc	Zn	+	+	

^aBased on data from Nykänen & Suomalainen (1983), supplemented by references cited in section 3