

PC	Measured mass (m/z)	Sum formula	Theoretical mass (m/z)	r	Tentative identification
1	117.091	$C_6H_{13}O_2^+$	117.0910	-0.80	Ethyl butanoate, ethyl-2-methylpropanoate (ethyl isobutyrate), hexanoic acid
	127.112	$C_8H_{15}O^+$	127.1120	-0.73	1-Octen-3-one
	145.123	$C_8H_{17}O_2^+$	145.1229	-0.73	Ethyl hexanoate, octanoic acid
	99.081	$C_6H_{11}O^+$	99.0804	-0.69	Hexanoic acid
	71.086	$C_5H_{11}^+$	71.0855	-0.61	3-Methyl-1-butanol, 3-methyl-3-buten-1-ol, pentan-1-ol
2	69.070	$C_5H_9^+$	69.0698	-0.62	2-Methyl-1,3-butadiene (isoprene)
	115.112	$C_7H_{15}O^+$	115.1117	-0.59	Heptan-2-one
	59.049	$C_3H_7O^+$	59.0491	-0.59	Propan-2-one (acetone)
	87.080	$C_5H_{11}O^+$	87.0804	-0.56	2-Methylbutanal, 3-methylbutanal, pentan-2-one
	101.097	$C_6H_{13}O^+$	101.0961	-0.55	Hexan-1-one, hexan-2-one, hexanal
3	42.034	$C_2H_4N^+$	42.0330	-0.70	Acetonitrile
	33.034	CH_5O^+	33.0335	-0.69	Methanol
	129.127	$C_8H_{17}O^+$	129.1270	0.66	Octan-1-one
	75.044	$C_3H_7O_2^+$	75.0440	-0.61	Propanoic acid
	143.143	$C_9H_{19}O^+$	143.1430	0.60	Nonan-2-one
4	109.070	$C_2^{13}CH_{10}O_3N^+$	109.0760	-0.65	2,6-Dimethylpyrazine
	95.017	$C_2H_7O_2S^+$	95.0160	-0.52	Methyldisulfanylmethane (dimethyl disulphide)
	75.044	$C_3H_7O_2^+$	75.0440	0.40	Propanoic acid
	61.028	$C_2H_5O_2^+$	61.0284	0.31	Acetic acid and fragment of acetate ester
	33.034	CH_5O^+	33.0335	0.31	Methanol
5	60.021	$C_2H_4O_2^+$	60.0205	-0.61	Acetic acid
	103.075	$C_5H_{11}O_2^+$	103.0754	-0.58	3-Methylbutanoic acid (isovaleric acid), ethyl (S)-2-hydroxypropanoate (ethyl lactate), pentanoic acid (valeric acid)
	105.091	$C_5H_{13}O_2^+$	105.0910	0.55	1,2-Pentanediol
	87.080	$C_5H_{11}O^+$	87.0804	0.53	2-Methylbutanal, 3-methylbutanal, pentan-2-one
	131.107	$C_7H_{15}O_2^+$	131.1067	-0.49	Ethyl-2-methylbutanoate, ethyl-3-methylbutanoate (ethyl isovalerate), heptanoic acid
6	71.049	$C_4H_7O^+$	71.0491	0.57	Butanoic acid
	41.039	$C_3H_5^+$	41.0386	-0.56	Alkyl fragment
	57.070	$C_4H_9^+$	57.0699	-0.46	Alkyl fragment
	90.063	$C_3^{[13]}CH_9O_2^+$	90.0631	0.41	2-Methylpropanoic acid (isobutyric acid), butanoic acid, ethyl acetate
	89.060	$C_4H_9O_2^+$	89.0597	0.41	3-Hydroxy-2-butanone (acetoin)
7	144.146	$C_8^{[13]}CH_{19}O^+$	144.1460	0.43	Nonan-2-one
	143.143	$C_9H_{19}O^+$	143.1430	0.42	Nonan-2-one
	45.033	$C_2H_5O^+$	45.0335	-0.38	Ethanal (acetaldehyde)
	41.039	$C_3H_5^+$	41.0386	-0.38	Alkyl fragment

	59.049	$C_3H_7O^+$	59.0491	-0.32	Propan-2-one (acetone)
8	105.071	$C_8H_9^+$	105.0700	-0.32	2-Phenylethanol/styrene
	143.143	$C_9H_{19}O^+$	143.1430	0.24	Nonan-2-one
	55.055	$C_4H_7^+$	55.0542	0.20	Butanal, heptanal, alkyl fragment
	61.028	$C_2H_5O_2^+$	61.0284	0.19	Acetic acid and fragment of acetate ester
	132.109	$C_6^{[13]}CH_{15}O_2^+$	132.1100	-0.18	Ethyl-2-methylbutanoate, ethyl-3-methylbutanoate (ethyl isovalerate), heptanoic acid
9	55.055	$C_4H_7^+$	55.0542	0.32	Butanal, heptanal, alkyl fragment
	71.086	$C_5H_{11}^+$	71.0855	-0.29	3-Methyl-1-butanol, 3-methyl-3-buten-1-ol, pentan-1-ol
	49.011	CH_5S^+	49.0106	-0.25	Methanethiol
	73.065	$C_4H_9O^+$	73.0648	0.25	Butan-2-one, butanal
	74.069	$C_3^{[13]}CH_9O^+$	73.0648	0.22	Butane-2,3-diol
10	45.033	$C_2H_5O^+$	45.0335	0.39	Ethanal (acetaldehyde)
	49.011	CH_5S^+	49.0106	-0.23	Methanethiol
	132.109	$C_6^{[13]}CH_{15}O_2^+$	132.1100	-0.21	Ethyl-2-methylbutanoate, ethyl-3-methylbutanoate (ethyl isovalerate), heptanoic acid
	69.070	$C_5H_9^+$	69.0698	-0.18	2-Methyl-1,3-butadiene (isoprene)
	99.081	$C_6H_{11}O^+$	99.0804	0.16	Hexanoic acid
