

**Appendix B. Identification information for compounds detected in urine.**

<b>ELUTION ORDER</b>	<b>COMPOUND NAME</b>	<b>DTXSID</b>	<b>PREFERRED_NAME</b>
1	1-Propanol	<a href="#">DTXSID2021739</a>	1-Propanol
2	2-Methyl-propanal	<a href="#">DTXSID9021635</a>	2-Methylpropanal
3	2-Butanone	<a href="#">DTXSID3021516</a>	Methyl ethyl ketone
4	2-Ethoxy-2-methylpropane	<a href="#">DTXSID0025604</a>	Ethyl T-butyl ether
5	2-Methyl-1-propanol	<a href="#">DTXSID0021759</a>	2-Methyl-1-propanol
6	Amylene Hydrate	<a href="#">DTXSID0041436</a>	2-Methyl-2-butanol
7	Isovaleraldehyde	<a href="#">DTXSID1021619</a>	3-Methylbutanal
8	1-Butanol	<a href="#">DTXSID1021740</a>	1-Butanol
9	2-Pentanone	<a href="#">DTXSID0021888</a>	2-Pentanone
10	Pentanal	<a href="#">DTXSID7021653</a>	Pentanal
11	3-Methyl-1-butanol	<a href="#">DTXSID3025469</a>	Isopentyl alcohol
12	4-Methyl-2-pentanone	<a href="#">DTXSID5021889</a>	4-Methyl-2-pentanone
13	Dimethyl disulfide	<a href="#">DTXSID4025117</a>	Methyl disulfide
14	3-Methyl-3-pentanol	<a href="#">DTXSID0021755</a>	3-Methyl-3-pentanol
15	Pyrrrole	<a href="#">DTXSID5021910</a>	Pyrrrole
16	4-Methyl-2-pentanol	<a href="#">DTXSID2026781</a>	4-Methyl-2-pentanol
17	1-Pentanol	<a href="#">DTXSID6021741</a>	1-Pentanol
18	Hexanal	<a href="#">DTXSID2021604</a>	Hexanal
19	Furfural	<a href="#">DTXSID1020647</a>	Furfural
20	2-Ethyl-1-butanol	<a href="#">DTXSID2041416</a>	2-Ethyl-1-butanol
21	1-Hexanol	<a href="#">DTXSID8021931</a>	1-Hexanol
22	4-Heptanone	<a href="#">DTXSID6047650</a>	4-Heptanone
23	Allyl isothiocyanate	<a href="#">DTXSID3020047</a>	Allyl isothiocyanate
24	Heptanal	<a href="#">DTXSID0021597</a>	Heptanal
25	1-Heptanol	<a href="#">DTXSID8021937</a>	1-Heptanol
26	Benzaldehyde	<a href="#">DTXSID8039241</a>	Benzaldehyde
27	Octanal	<a href="#">DTXSID3021643</a>	Octanal
28	Carvone	<a href="#">DTXSID8047426</a>	dl-Carvone

<b>EPA CHEMISTRY DASHBOARD INPUT</b>	<b>FOUND_BY</b>	<b>RETENTION TIME (min)</b>	<b>SIM ION (amu)</b>
1-Propanol	Approved Name	5.016	59
2-Methyl-propanal	Synonym	5.042	72
2-Butanone	Expert Validated Synonym	5.427	72
2-Ethoxy-2-methylpropane	Synonym from Valid Source	5.756	59
2-Methyl-1-propanol	Approved Name	5.809	43
Amylene Hydrate	Synonym from Valid Source	6.001	59
Isovaleraldehyde	Expert Validated Synonym	6.245	44
1-Butanol	Approved Name	6.351	56
2-Pentanone	Approved Name	6.766	43
Pentanal	Approved Name	6.939	44
3-Methyl-1-butanol	Synonym from Valid Source	7.642	55
4-Methyl-2-pentanone	Approved Name	7.759	43
Dimethyl disulfide	Synonym from Valid Source	7.957	94
3-Methyl-3-pentanol	Approved Name	8.01	73
Pyrrole	Approved Name	8.071	67
4-Methyl-2-pentanol	Approved Name	8.106	45
1-Pentanol	Approved Name	8.274	42
Hexanal	Approved Name	8.986	56
Furfural	Approved Name	9.742	96
2-Ethyl-1-butanol	Approved Name	9.837	43
1-Hexanol	Approved Name	10.42	56
4-Heptanone	Approved Name	10.54	71
Allyl isothiocyanate	Approved Name	10.824	99
Heptanal	Approved Name	11.145	70
1-Heptanol	Approved Name	12.501	70
Benzaldehyde	Approved Name	12.527	106
Octanal	Approved Name	13.205	43
Carvone	Synonym from Valid Source	17.76	82

CONFIRMATION IONS (amu)	R <sup>2</sup>
31, 42	0.993
43	0.989
43, 39	0.998
87	0.994
33	0.994
73	0.991
58	0.995
41	0.995
86	0.989
58	0.993
7	0.997
58, 100	0.997
79	0.987
55	0.994
39	0.992
69	0.993
55	0.988
72	0.987
95	0.99
70	0.984
43, 69	0.984
114	0.999
39	0.996
43	0.999
56	0.992
105	0.997
57	0.996
54	0.983

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