

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX051920\
 Data File : VX016339.D
 Acq On : 19 May 2020 16:58
 Operator : JC/SP
 Sample : L2673-03
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 104

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.160	9	12	20	rVB2	50089	46774	3.72%	0.484%
2	1.471	60	63	69	rBV	15569	18383	1.46%	0.190%
3	2.331	198	204	213	rVB	69828	112727	8.95%	1.167%
4	2.416	213	218	223	rBV	22062	33895	2.69%	0.351%
5	2.575	236	244	259	rVB	66681	126326	10.03%	1.307%
6	3.008	308	315	325	rVB2	8986	21161	1.68%	0.219%
7	3.916	456	464	477	rBV3	6964	21281	1.69%	0.220%
8	4.300	516	527	542	rBV	71425	201650	16.02%	2.087%
9	4.642	575	583	600	rBV3	12307	41201	3.27%	0.426%
10	5.471	708	719	731	rBV	122406	350580	27.85%	3.628%
11	5.629	733	745	760	rVB	227292	639954	50.83%	6.623%
12	6.032	801	811	824	rBV	135883	363222	28.85%	3.759%
13	6.836	932	943	954	rBV	345859	838431	66.60%	8.677%
14	7.275	1006	1015	1024	rBV3	5474	14731	1.17%	0.152%
15	8.696	1241	1248	1255	rBV	750708	1181137	93.82%	12.224%
16	9.043	1299	1305	1317	rVB2	16873	30503	2.42%	0.316%
17	9.202	1326	1331	1340	rBV	15988	27950	2.22%	0.289%
18	10.098	1469	1478	1489	rBV	806121	1111139	88.26%	11.499%
19	10.195	1489	1494	1498	rBV	35961	50172	3.99%	0.519%
20	10.342	1513	1518	1524	rVB	11440	17756	1.41%	0.184%
21	10.543	1546	1551	1561	rVB	103979	128327	10.19%	1.328%
22	10.720	1576	1580	1586	rVB	27213	35256	2.80%	0.365%
23	10.793	1587	1592	1601	rBV	85163	126930	10.08%	1.314%
24	11.122	1640	1646	1651	rBV	680803	855494	67.95%	8.854%
25	11.171	1651	1654	1659	rVB	37537	47670	3.79%	0.493%
26	11.421	1687	1695	1704	rBV2	7914	24510	1.95%	0.254%
27	11.610	1721	1726	1729	rBV	54533	71010	5.64%	0.735%
28	11.646	1729	1732	1738	rVV3	38892	61509	4.89%	0.637%
29	11.720	1738	1744	1750	rVB	58045	75672	6.01%	0.783%
30	11.793	1752	1756	1761	rVB	17927	22798	1.81%	0.236%
31	11.866	1761	1768	1771	rBV2	17567	27730	2.20%	0.287%
32	11.909	1771	1775	1782	rVV	145847	202771	16.11%	2.099%
33	12.006	1786	1791	1796	rVV2	48618	87196	6.93%	0.902%
34	12.061	1796	1800	1807	rVV	905759	1105114	87.78%	11.437%

LSC Area Percent Report

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Integration Parameters: RTEINT.P

Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

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Title : SW846 8260

35	12.256	1827	1832	1844	rBV	932820	1258959	100.00%	13.029%
36	12.341	1844	1846	1859	rVB6	19537	54338	4.32%	0.562%
37	12.604	1882	1889	1895	rBV5	10930	27381	2.17%	0.283%
38	12.847	1924	1929	1932	rVB4	11024	18085	1.44%	0.187%
39	13.622	2051	2056	2065	rBV	7664	14626	1.16%	0.151%
40	13.792	2080	2084	2086	rVV2	11587	17076	1.36%	0.177%
41	13.817	2086	2088	2092	rVV	10715	15129	1.20%	0.157%
42	13.884	2094	2099	2105	rVV	39244	57506	4.57%	0.595%
43	13.951	2106	2110	2127	rVB	38225	63664	5.06%	0.659%
44	15.036	2283	2288	2297	rBV7	9511	14891	1.18%	0.154%

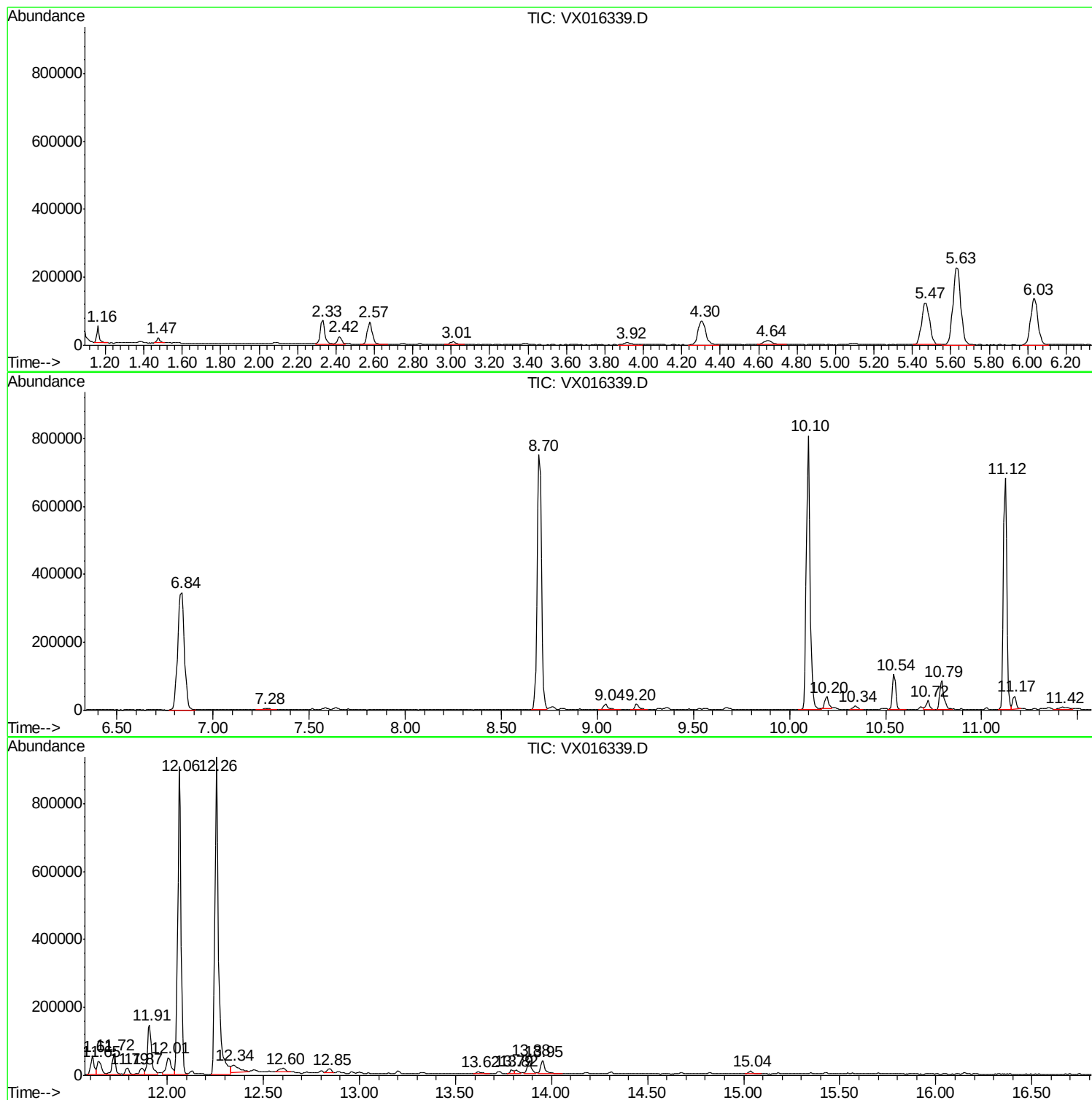
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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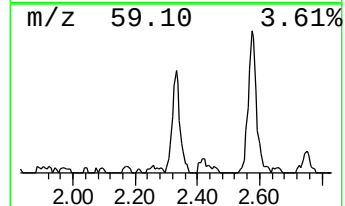
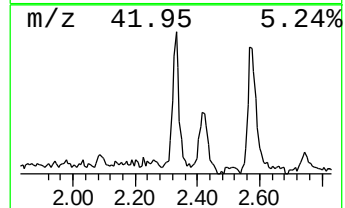
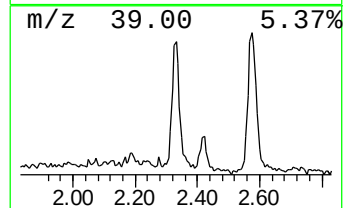
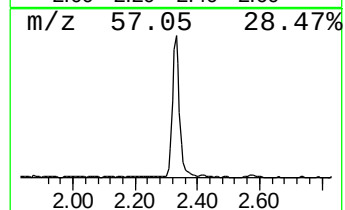
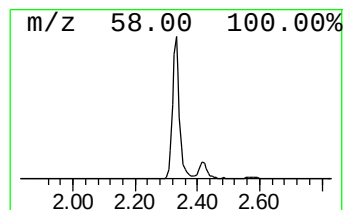
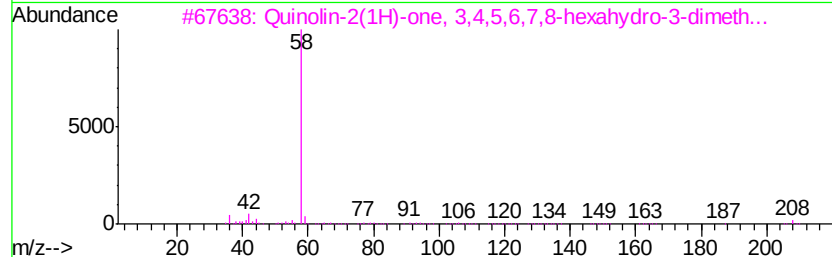
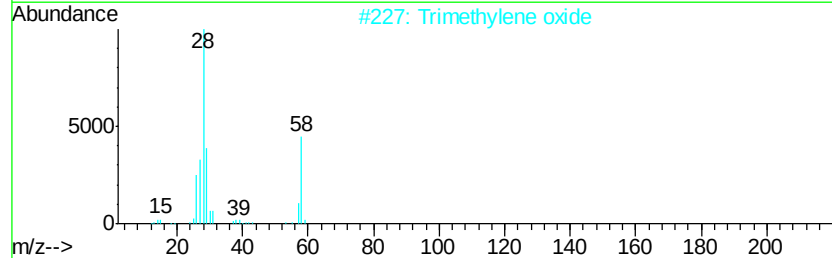
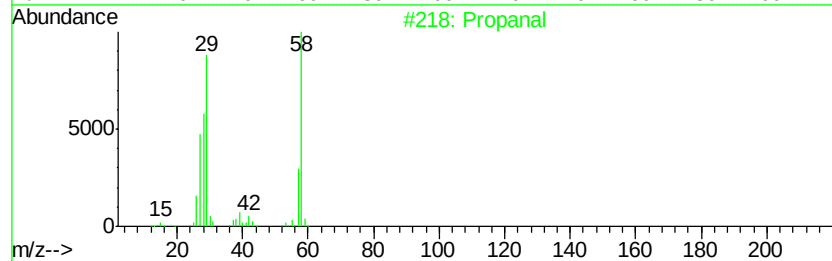
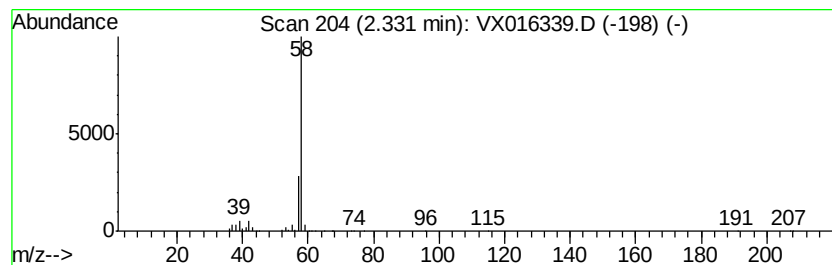
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	8.81 ug/l	112727	Pentafluorobenzene	5.63

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal		58	C3H6O	000123-38-6	78
2	Trimethylene oxide		58	C3H6O	000503-30-0	64
3	Quinolin-2(1H)-one, 3,4,5,6,7,8-...		208	C12H20N2O	1000259-95-6	40
4	.alpha.-Pinene, 10-(dimethylamin...		193	C13H23N	015063-97-5	9
5	Propylene oxide		58	C3H6O	000075-56-9	7



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ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampled :
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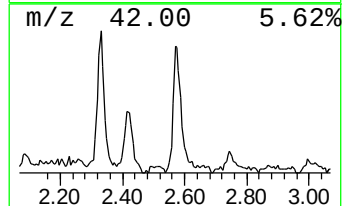
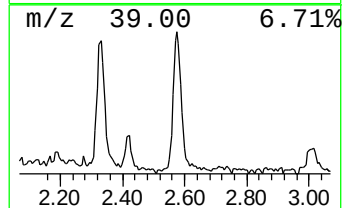
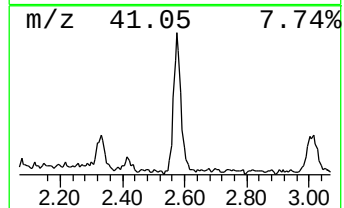
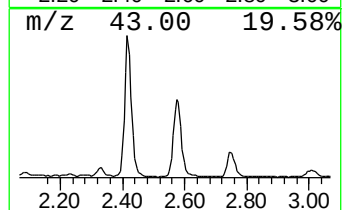
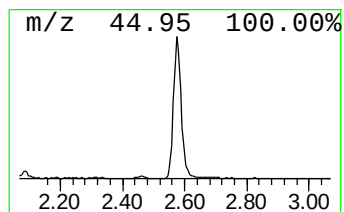
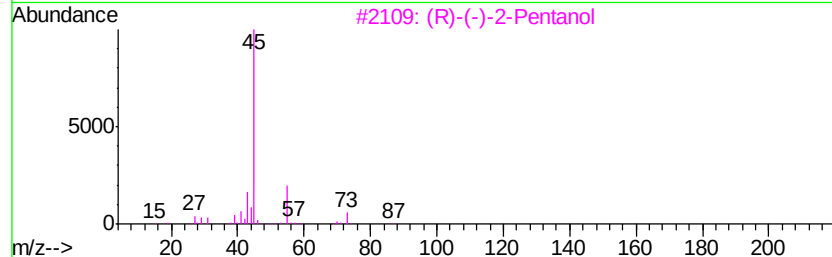
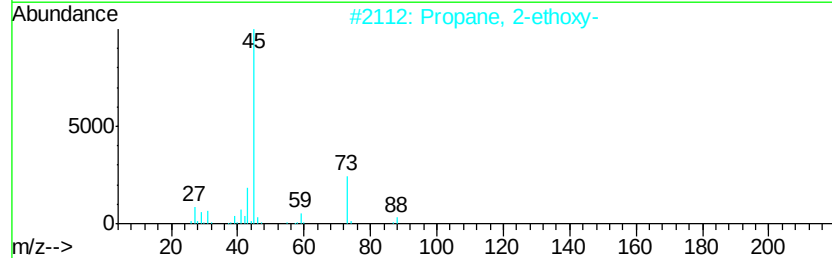
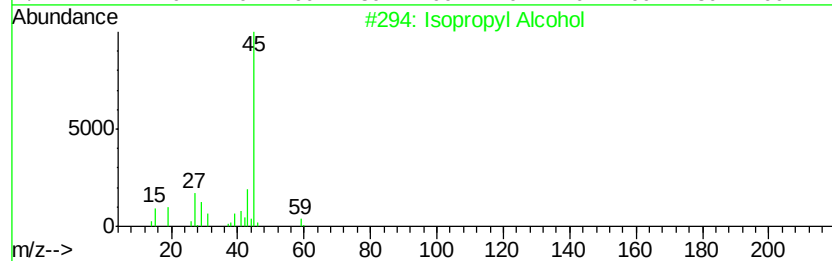
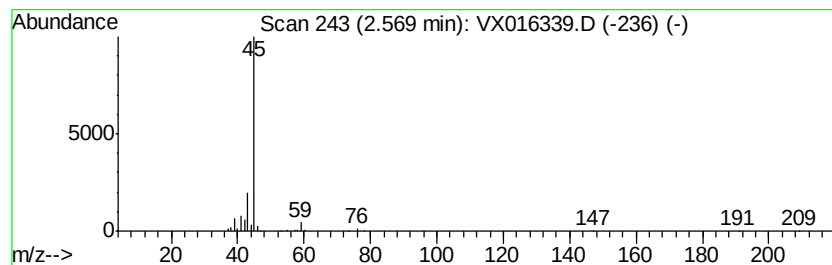
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.57	9.87 ug/l	126326	Pentafluorobenzene	5.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2		Propane, 2-ethoxy-	88	C5H12O	000625-54-7	56
3		(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	9
4		(R)-(-)-3-Methyl-2-butanol	88	C5H12O	001572-93-6	9
5		2-Pentanol	88	C5H12O	006032-29-7	9



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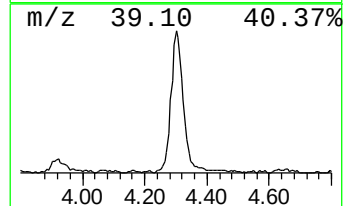
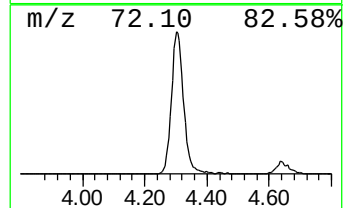
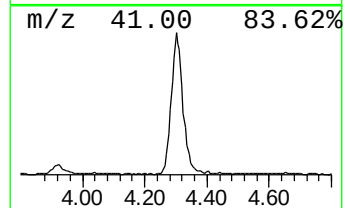
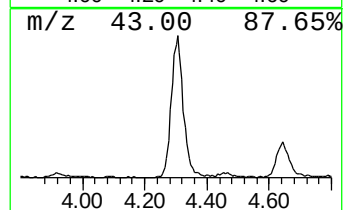
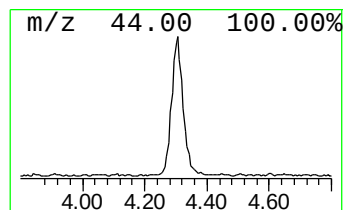
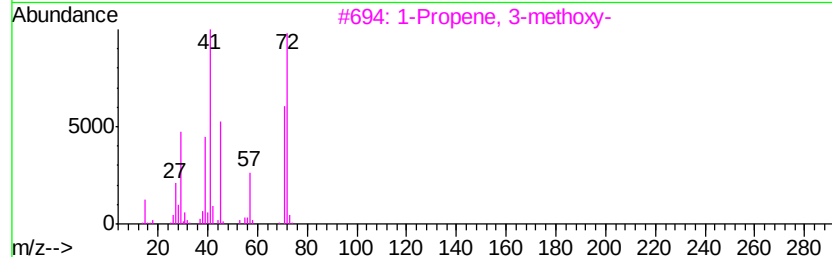
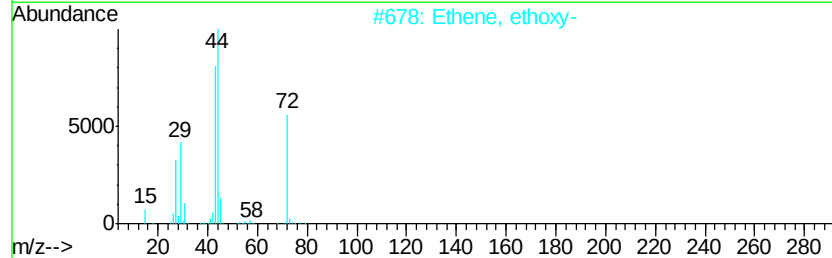
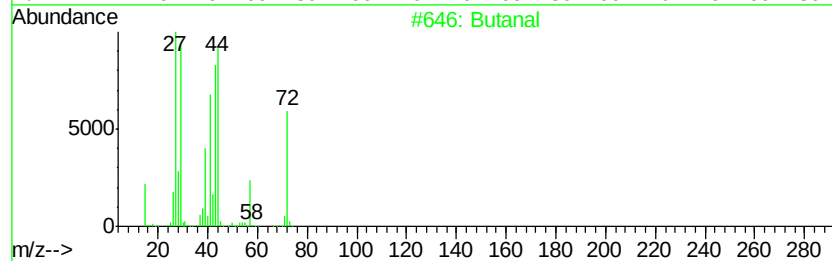
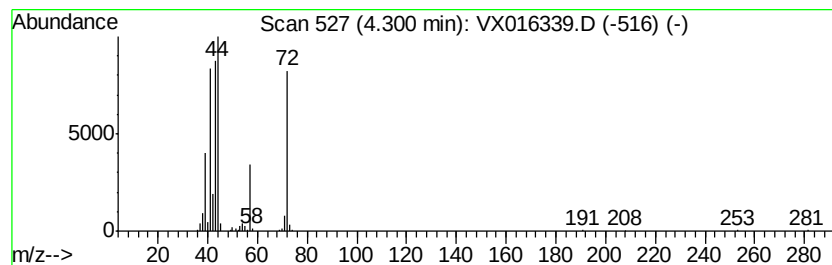
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.30	15.76 ug/l	201650	Pentafluorobenzene	5.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanal	72	C4H8O	000123-72-8	91
2		Ethene, ethoxy-	72	C4H8O	000109-92-2	50
3		1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43
4		Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
5		L-Alanine, N-formyl-	117	C4H7NO3	010512-86-4	33



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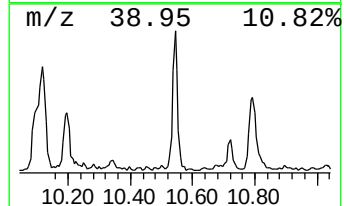
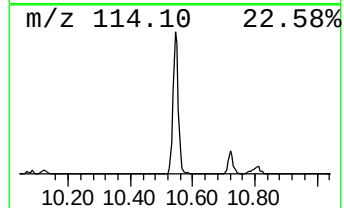
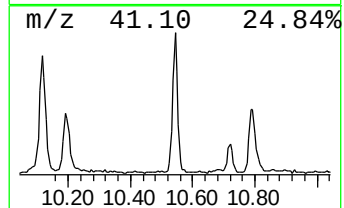
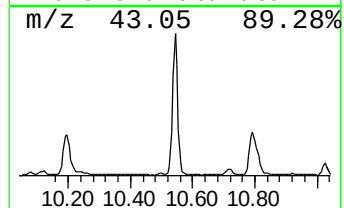
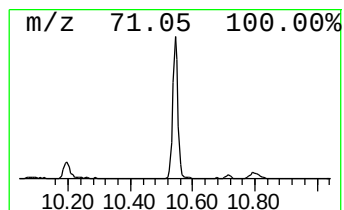
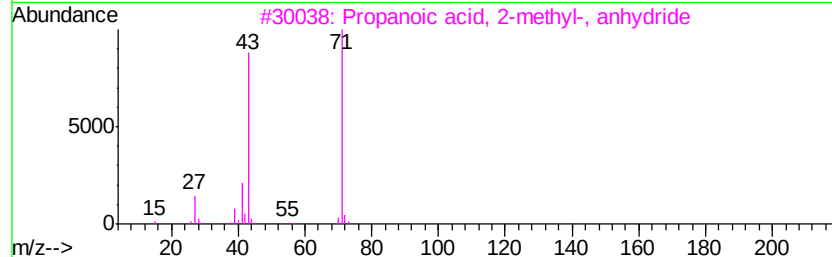
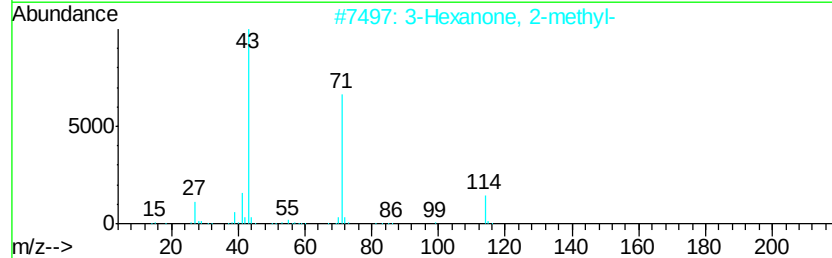
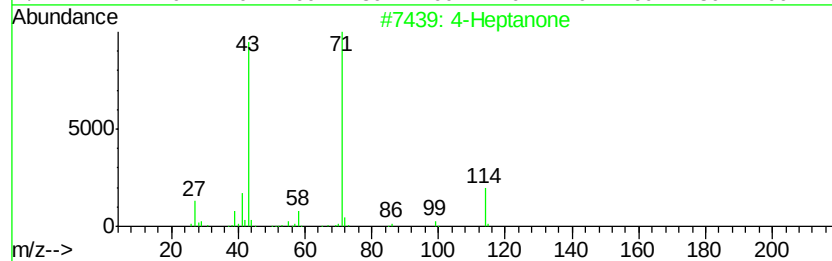
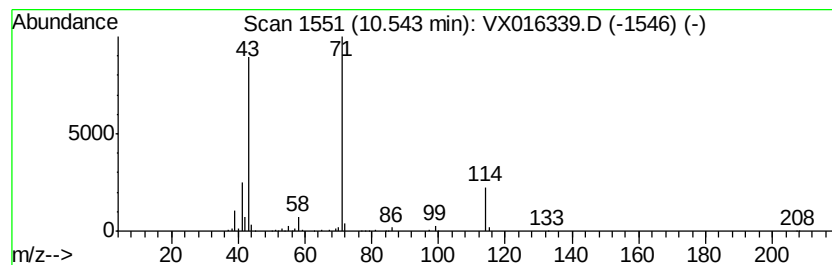
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 4-Heptanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.54	5.77 ug/l	128327	Chlorobenzene-d5	10.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Heptanone	114	C7H14O	000123-19-3	91
2		3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	78
3		Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	59
4		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	45
5		Pentane, 3-bromo-	150	C5H11Br	001809-10-5	42



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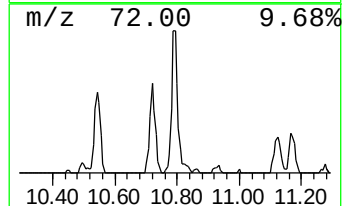
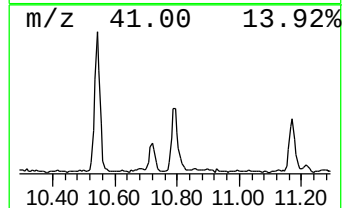
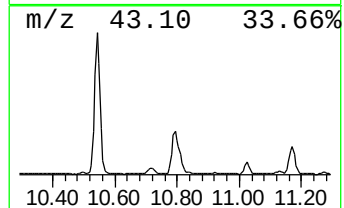
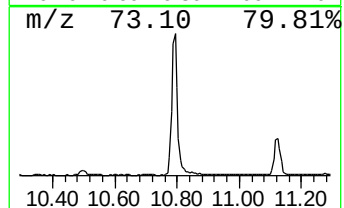
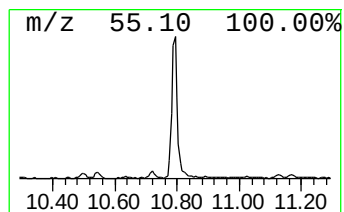
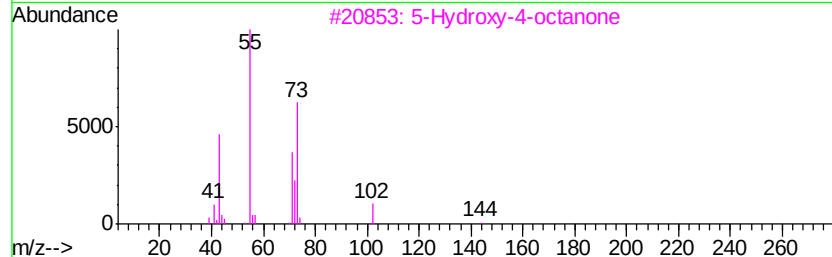
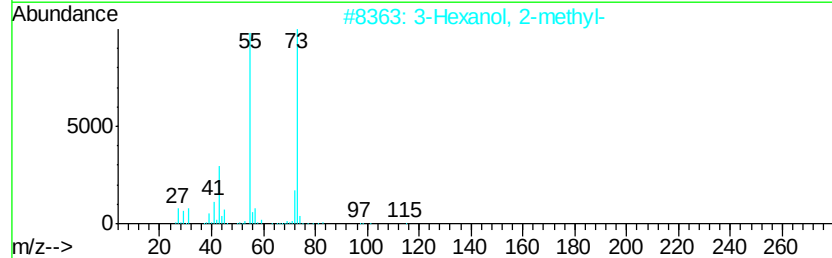
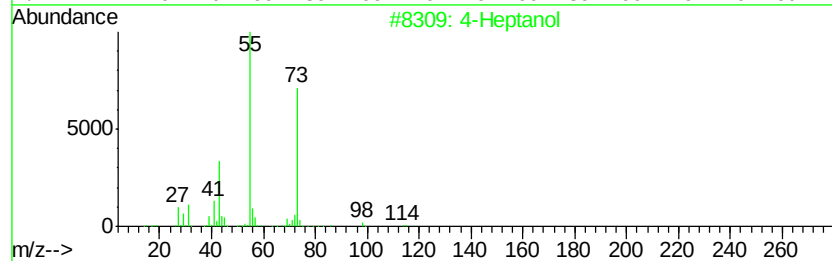
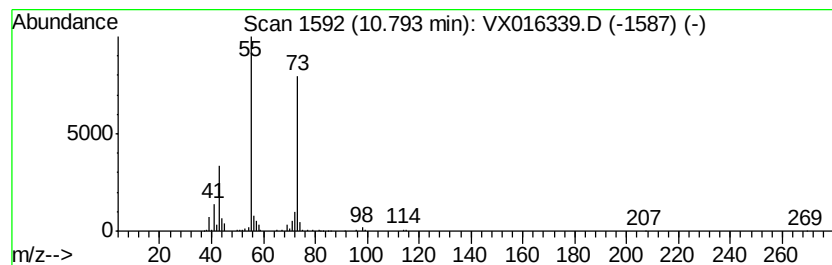
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 5 4-Heptanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.79	5.71 ug/l	126930	Chlorobenzene-d5	10.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Heptanol	116	C7H16O	000589-55-9	72
2		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	59
3		5-Hydroxy-4-octanone	144	C8H16O2	000496-77-5	47
4		1-Hepten-4-ol	114	C7H14O	003521-91-3	40
5		1-Heptene, 5-methoxy-4-methyl-	142	C9H18O	054004-21-6	28



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX051920\
Data File : VX016339.D
Acq On : 19 May 2020 16:58
Operator : JC/SP
Sample : L2673-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
104

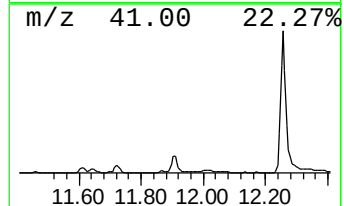
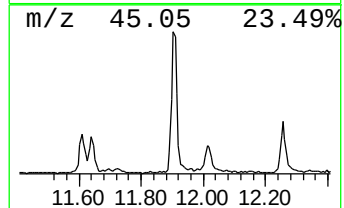
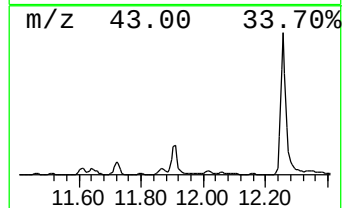
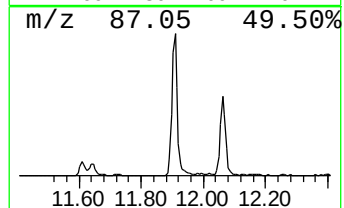
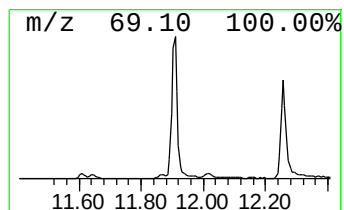
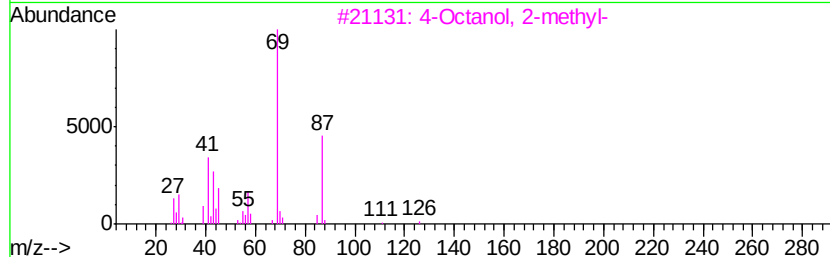
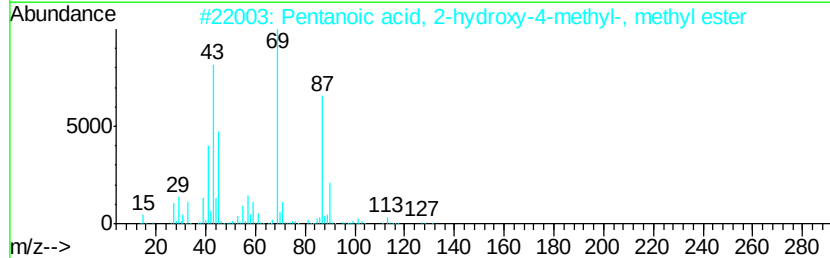
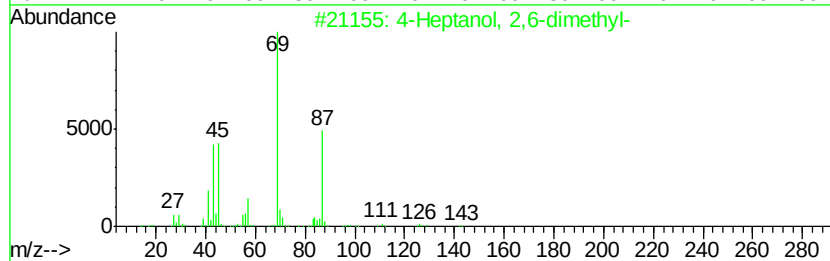
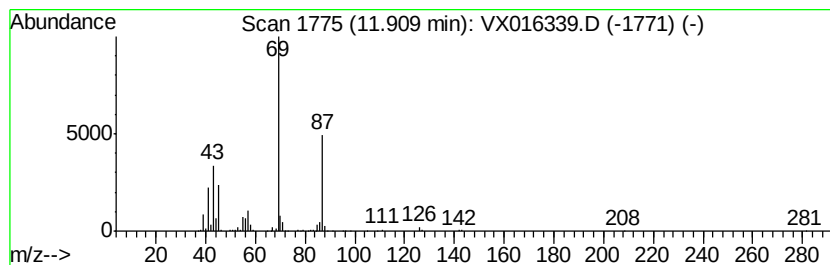
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 4-Heptanol, 2,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	9.17 ug/l	202771	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	83
2		Pentanoic acid, 2-hydroxy-4-meth...	146	C7H14O3	040348-72-9	72
3		4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	72
4		5-Nonanol	144	C9H20O	000623-93-8	72
5		4-Octanol	130	C8H18O	000589-62-8	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX051920\
 Data File : VX016339.D
 Acq On : 19 May 2020 16:58
 Operator : JC/SP
 Sample : L2673-03
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 19 Sample Multiplier: 1

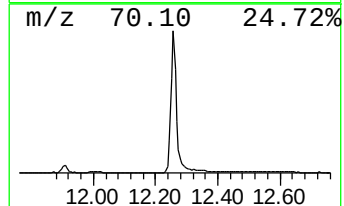
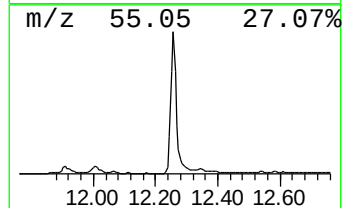
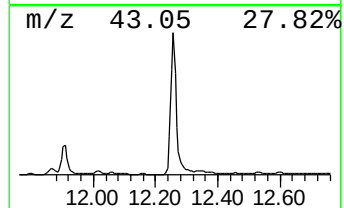
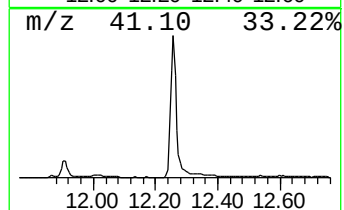
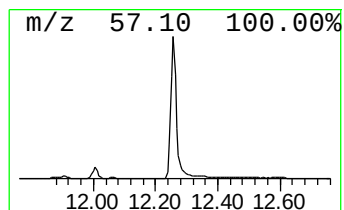
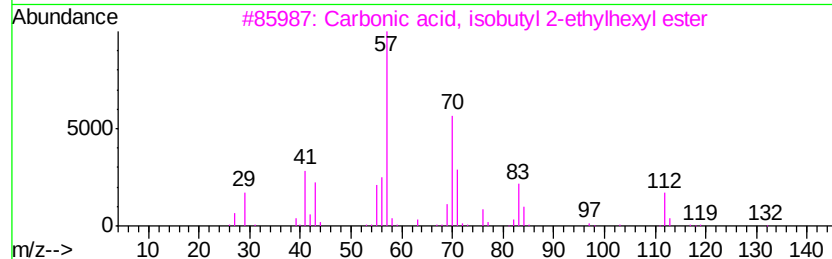
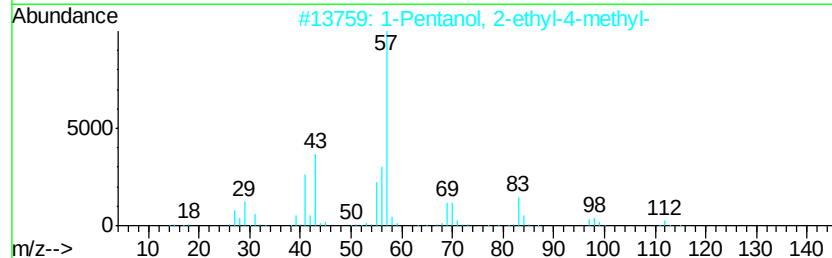
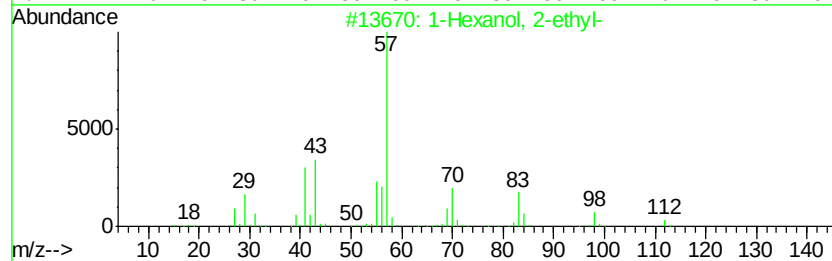
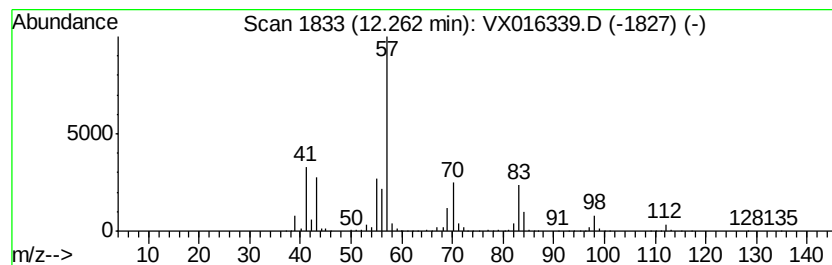
Instrument :
 MSVOA_X
 ClientSampleId :
 104

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
 Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.26	56.96 ug/l	1258960	1,4-Dichlorobenzene-d4	12.06	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	53
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX051920\
Data File : VX016339.D
Acq On : 19 May 2020 16:58
Operator : JC/SP
Sample : L2673-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
104

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X050420W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanal	2.33	8.8	ug/l	112727	1	5.63	639954	50.0
Isopropyl Alcohol	2.57	9.9	ug/l	126326	1	5.63	639954	50.0
Butanal	4.30	15.8	ug/l	201650	1	5.63	639954	50.0
4-Heptanone	10.54	5.8	ug/l	128327	3	10.10	1111140	50.0
4-Heptanol	10.79	5.7	ug/l	126930	3	10.10	1111140	50.0
4-Heptanol, 2,6-d...	11.91	9.2	ug/l	202771	4	12.06	1105110	50.0
1-Hexanol, 2-ethyl-	12.26	57.0	ug/l	1258960	4	12.06	1105110	50.0