LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
Data File : VX021209.D
Acq On : 15 Mar 2021 18:54
Operator : JC/MD
Sample : M1647-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : COMP1-41730:31

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

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Title : SW846 8260

Signal : TIC: VX021209.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.163	9	13	19	rBV2	22019	20684	4.42%	0.395%
2	1.281	30	33	37	rBV2	6139	6954	1.48%	0.133%
3	1.381	46	50	55	rBV2	4742	7297	1.56%	0.139%
4	1.475	62	66	72	rBV	30604	33840	7.23%	0.647%
5	1.569	77	82	84	rBV2	5623	7226	1.54%	0.138%
6	1.605	84	88	91	rVB3	5018	7166	1.53%	0.137%
7	2.099	165	172	181	rBV	29975	46524	9.93%	0.889%
8	2.334	207	212	220	rVB2	2850	4720	1.01%	0.090%
9	2.422	220	227	232	rBV	28417	48116	10.27%	0.919%
10	2.458	232	233	245	rVB3	5294	7369	1.57%	0.141%
11	2.581	245	254	260	rBV	8257	15665	3.34%	0.299%
12	2.752	275	283	293	rBV	26652	47062	10.05%	0.899%
13	3.011	319	327	336	rBV	16264	35863	7.66%	0.685%
14	3.758	442	454	466	rBV	33369	95154	20.32%	1.818%
15	4.076	498	508	516	rBV5	2076	5811	1.24%	0.111%
16	4.299	532	546	560	rBV	38526	116364	24.84%	2.223%
17	4.634	596	603	615	rBV	4173	11584	2.47%	0.221%
18	5.464	734	744	760	rBV	56783	161012	34.38%	3.076%
19	5.629	760	772	786	rBV2	84915	235965	50.38%	4.509%
20	6.035	828	841	848	rBV	65475	174380	37.23%	3.332%
21	6.111	848	854	873	rVB2	38729	111873	23.89%	2.138%
22	6.829	965	976	989	rBV	145140	346581	74.00%	6.622%
23	7.270	1044	1051	1061	rBV	14337	32825	7.01%	0.627%
24	7.635	1108	1113	1120	rVB	4014	7370	1.57%	0.141%
25	7.717	1120	1127	1138	rVB3	2091	5799	1.24%	0.111%
26	8.617	1274	1280	1285	rBV2	2705	4776	1.02%	0.091%
27	8.694	1285	1293	1299	rBV	300350	468371	100.00%	8.949%
28	8.764	1299	1305	1312	rVB	157298	242918	51.86%	4.641%
29	9.064	1350	1356	1363	rBV3	2656	5282	1.13%	0.101%
30	9.276	1386	1392	1401	rBV	17236	29932	6.39%	0.572%
31	9.482	1421	1427	1430	rBV3	7304	12314	2.63%	0.235%
32	9.529	1430	1435	1444	rVB	125119	184298	39.35%	3.521%
33	10.094	1525	1531	1535	rBV	329462	439248	93.78%	8.393%
34	10.135	1535	1538	1543	rVV	59038	79633	17.00%	1.522%
35	10.194	1543	1548	1552	rVV	38633	57221	12.22%	1.093%
36	10.235	1552	1555	1563	rVB	9697	14831	3.17%	0.283%

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ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : COMP1-41730:31

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Title : SW846 8260

37	10.341	1568	1573	1579	rVB	34933	48520	10.36%	0.927%
38	10.447	1584	1591	1596	rBV3	29611	50213	10.72%	0.959%
39	10.606	1613	1618	1626	rBV3	8539	13428	2.87%	0.257%
40	10.682	1626	1631	1640	rBV3	22177	39089	8.35%	0.747%
41	10.788	1645	1649	1653	rBV	19748	27779	5.93%	0.531%
42	10.824	1653	1655	1662	rVB2	6456	8720	1.86%	0.167%
43	10.894	1662	1667	1672	rBV4	11034	19110	4.08%	0.365%
44	10.947	1672	1676	1681	rVB2	11041	14424	3.08%	0.276%
45	11.118	1697	1705	1711	rBV	265616	348523	74.41%	6.659%
46	11.171	1711	1714	1720	rVB2	9974	12857	2.75%	0.246%
47	11.324	1734	1740	1743	rBV3	7476	13073	2.79%	0.250%
48	11.353	1743	1745	1748	rVV4	7610	12049	2.57%	0.230%
49	11.388	1748	1751	1758	rVV2	14103	22716	4.85%	0.434%
50	11.459	1758	1763	1766	rVV4	4623	8411	1.80%	0.161%
51	11.612	1784	1789	1791	rBV2	13253	18501	3.95%	0.353%
52	11.641	1791	1794	1798	rVB2	7768	10353	2.21%	0.198%
53	11.724	1803	1808	1816	rVV2	70245	107773	23.01%	2.059%
54	11.788	1816	1819	1824	rVV	8921	11271	2.41%	0.215%
55	11.847	1824	1829	1831	rVV4	4291	6387	1.36%	0.122%
56	11.906	1831	1839	1847	rVV	30948	56425	12.05%	1.078%
57	11.988	1850	1853	1856	rVV	12821	18735	4.00%	0.358%
58	12.024	1856	1859	1861	rVV	31358	40667	8.68%	0.777%
59	12.059	1861	1865	1874	rVV	338954	419355	89.53%	8.013%
60	12.253	1893	1898	1909	rBV	252943	367539	78.47%	7.023%
61	12.341	1910	1913	1919	rVV7	17159	33095	7.07%	0.632%
62	12.394	1919	1922	1927	rVV	7715	12835	2.74%	0.245%
63	12.453	1927	1932	1939	rVB	26694	34782	7.43%	0.665%
64	12.630	1959	1962	1970	rVB7	5056	8112	1.73%	0.155%
65	12.730	1975	1979	1986	rVB7	3586	8117	1.73%	0.155%
66	12.836	1986	1997	2003	rBV9	7758	18708	3.99%	0.357%
67	12.994	2021	2024	2029	rVB3	4708	7167	1.53%	0.137%
68	13.324	2077	2080	2085	rVB4	4743	6318	1.35%	0.121%
69	13.459	2098	2103	2108	rVB6	5682	9118	1.95%	0.174%
70	13.636	2127	2133	2144	rBV6	10993	28039	5.99%	0.536%
71	13.771	2151	2156	2159	rBV5	4826	7354	1.57%	0.141%
72	13.818	2159	2164	2171	rVV2	82131	114903	24.53%	2.195%
73	13.883	2171	2175	2183	rVV2	13706	22890	4.89%	0.437%
74	13.953	2183	2187	2198	rVB	13333	21250	4.54%	0.406%
75	14.512	2278	2282	2293	rVB2	14947	23065	4.92%	0.441%
76	14.612	2293	2299	2304	rBV	7982	10251	2.19%	0.196%

LSC Area Percent Report

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ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : COMP1-41730:31

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Title : SW846 8260

77	14.677	2304	2310	2315	rVB	13345	17510	3.74%	0.335%
78	14.818	2330	2334	2342	rBV	11010	14434	3.08%	0.276%
79	16.024	2532	2539	2548	rBV5	4029	7814	1.67%	0.149%

Sum of corrected areas: 5233708

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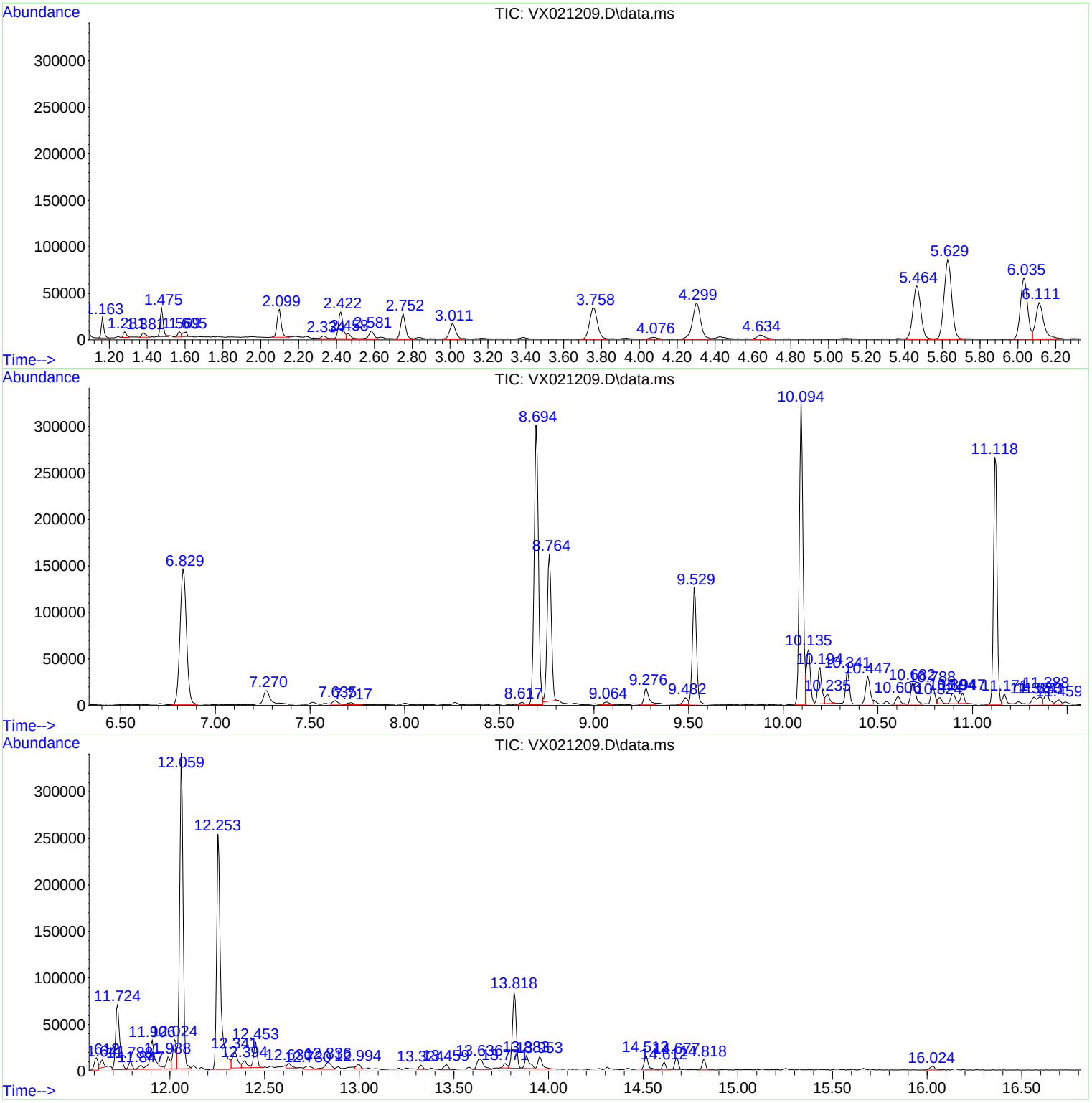
Operator : JC/MD
Sample : M1647-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP1-41730:31

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
Data File : VX021209.D
Acq On : 15 Mar 2021 18:54
Operator : JC/MD
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ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : COMP1-41730:31

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

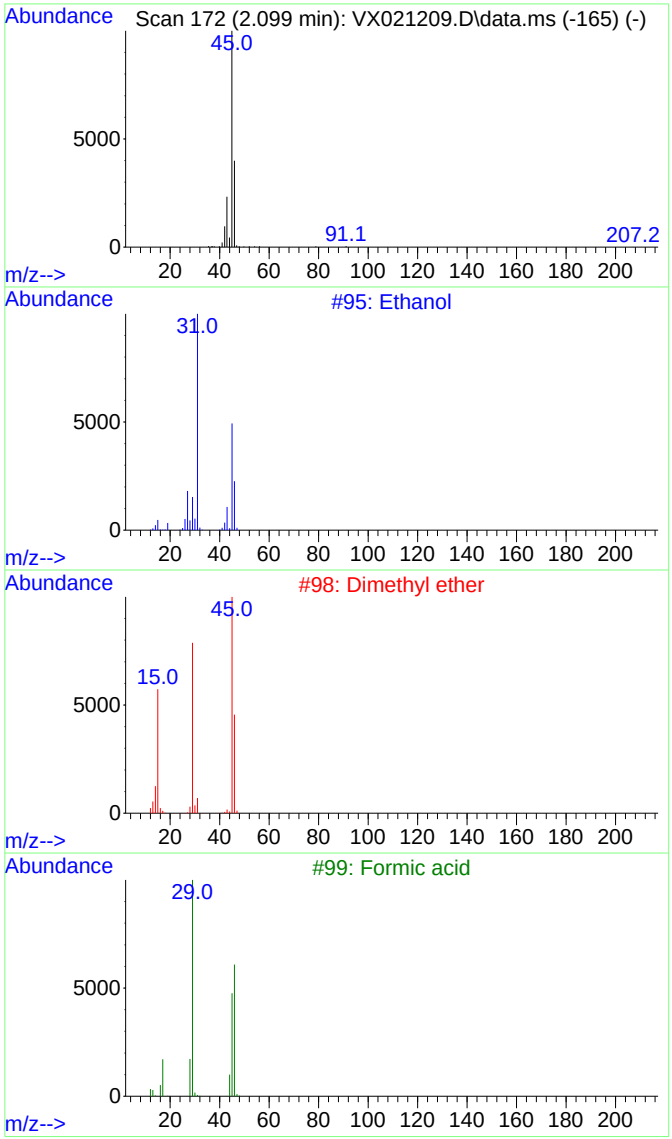
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

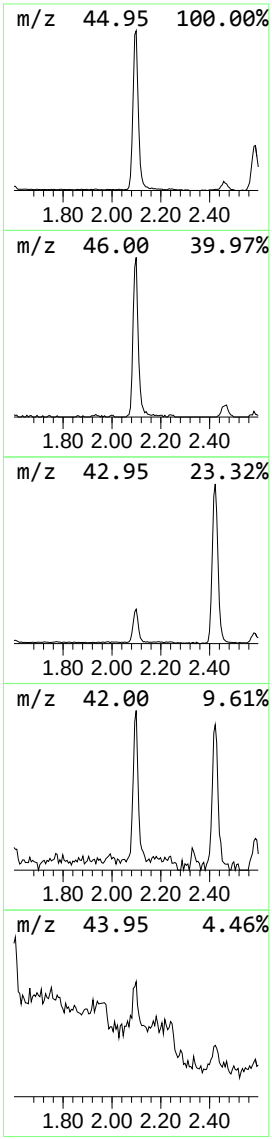
****

Peak Number 2 unknown2.099 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.099	9.86 ug/l	46524	Pentafluorobenzene	5.623

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	43
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Formic acid	46	CH2O2	000064-18-6	4
4	Methoxyacetic acid, pentyl ester	160	C8H16O3	168920-35-2	4
5	Oxalic acid	90	C2H2O4	000144-62-7	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
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Operator : JC/MD
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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP1-41730:31

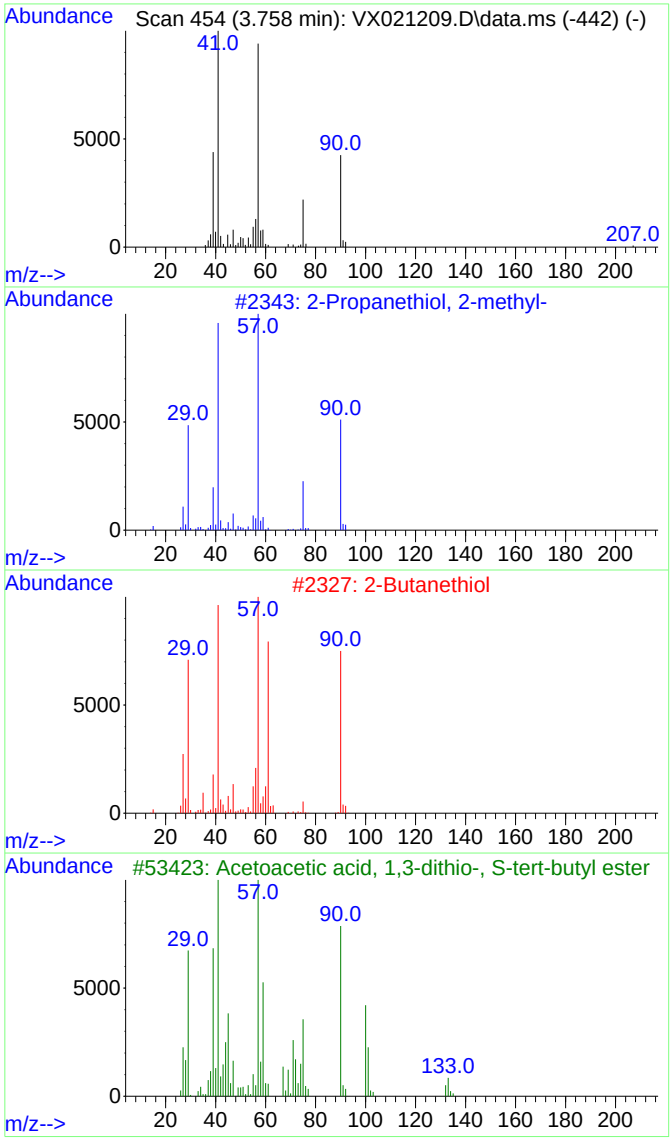
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

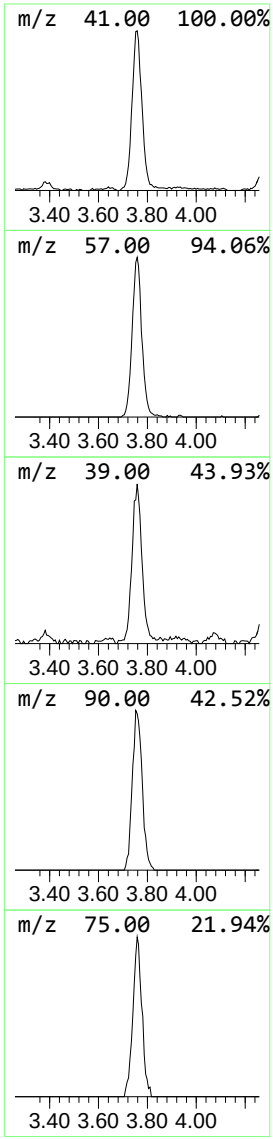
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanethiol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.758	20.16 ug/l	95154	Pentafluorobenzene	5.623

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	64
2	2-Butanethiol	90	C4H10S	000513-53-1	38
3	Acetoacetic acid, 1,3-dithio-, S...	190	C8H14OS2	020383-06-6	38
4	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	32
5	Propanamide, 2,2-dimethyl-	101	C5H11NO	000754-10-9	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
Data File : VX021209.D
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Operator : JC/MD
Sample : M1647-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP1-41730:31

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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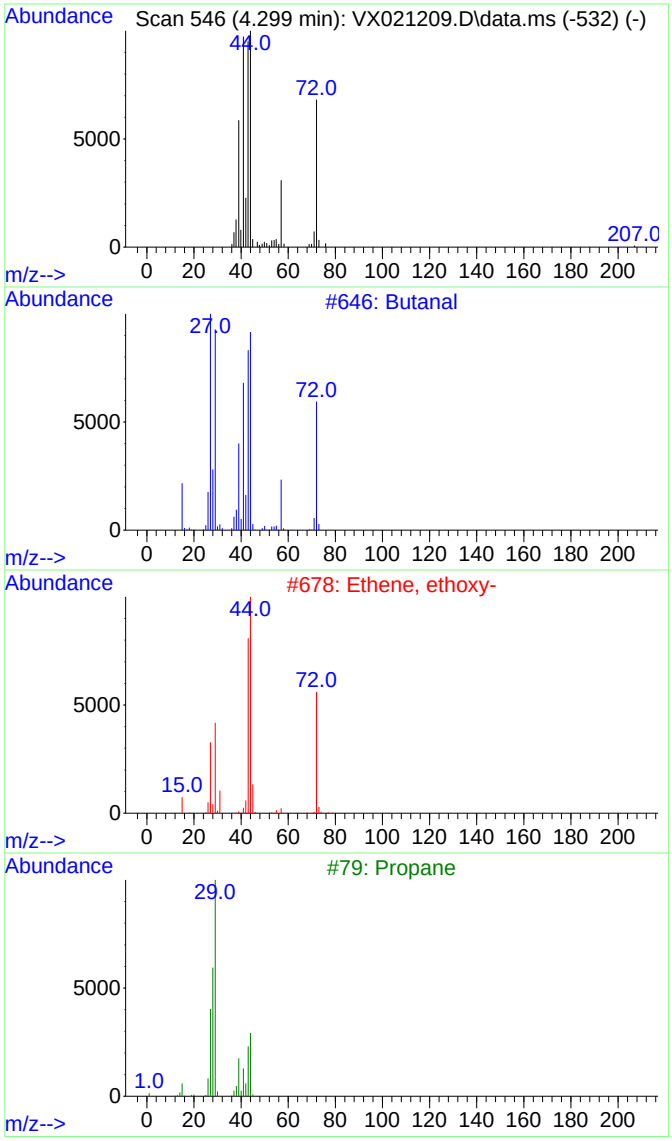
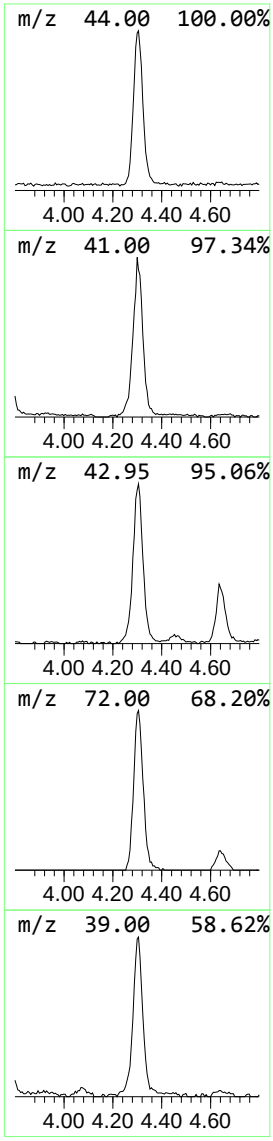
****
Peak Number 4 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.299	24.66 ug/l	116364	Pentafluorobenzene	5.623

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	47
3	Propane	44	C3H8	000074-98-6	43
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
5	Methacrolein	70	C4H6O	000078-85-3	27





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Instrument : MSVOA_X
ClientSampleId : COMP1-41730:31

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

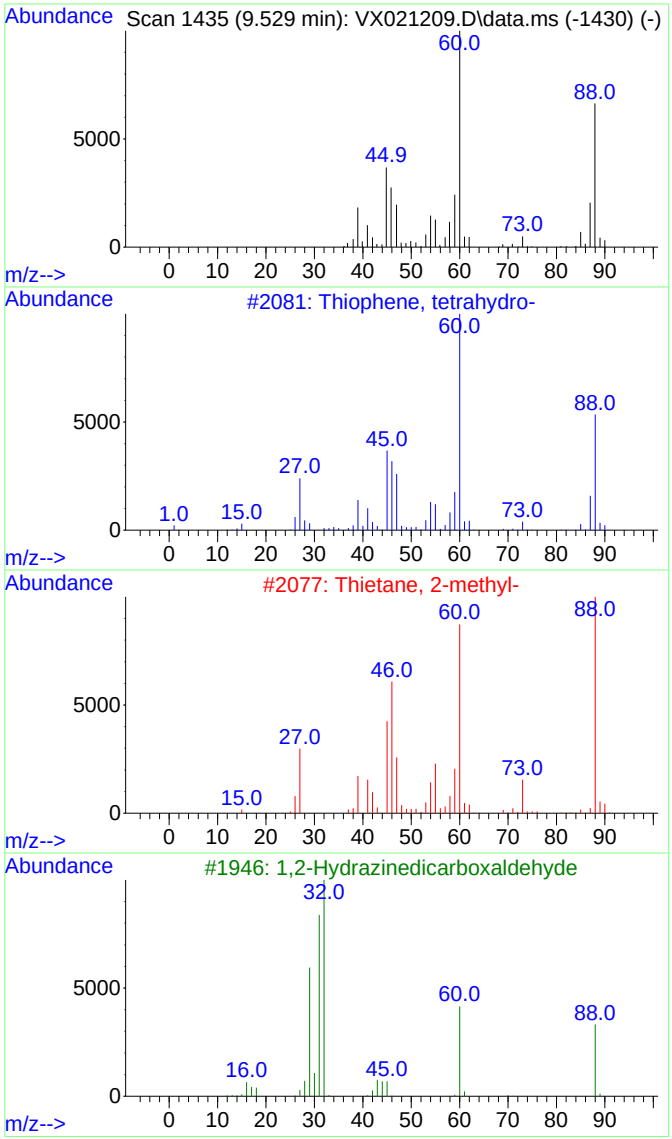
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

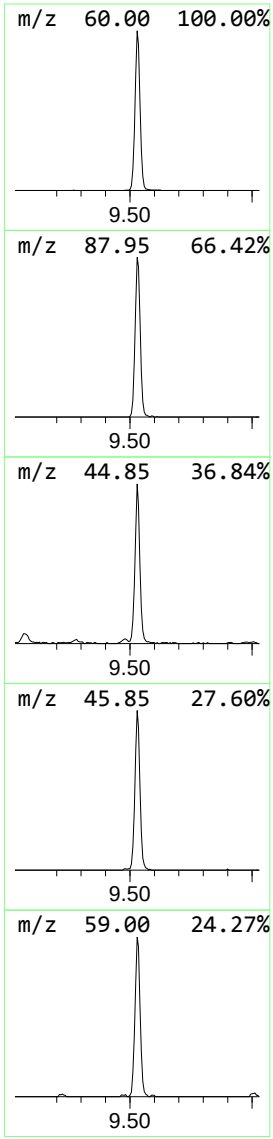
****

Peak Number 5 Thiophene, tetrahydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.529	20.98 ug/l	184298	Chlorobenzene-d5	10.094

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-	88	C4H8S	000110-01-0	97
2	Thietane, 2-methyl-	88	C4H8S	017837-41-1	74
3	1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	43
4	Ethylvinyl sulfide	88	C4H8S	000627-50-9	38
5	Ethanol, 2-mercapto-	78	C2H6OS	000060-24-2	25





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Operator : JC/MD
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ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP1-41730:31

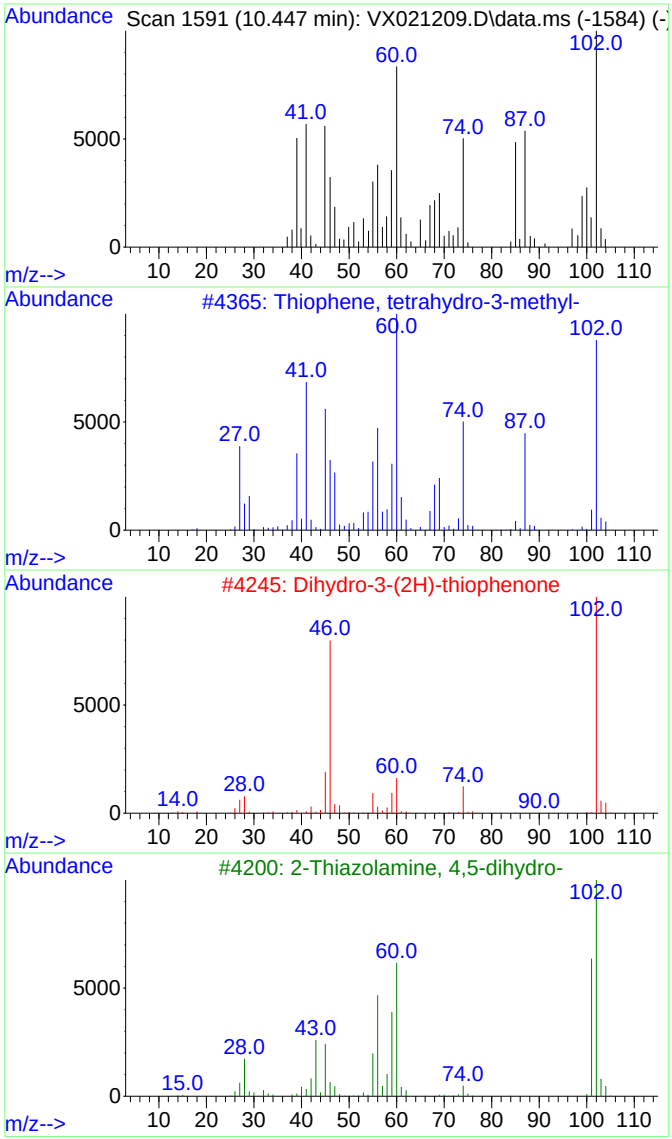
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

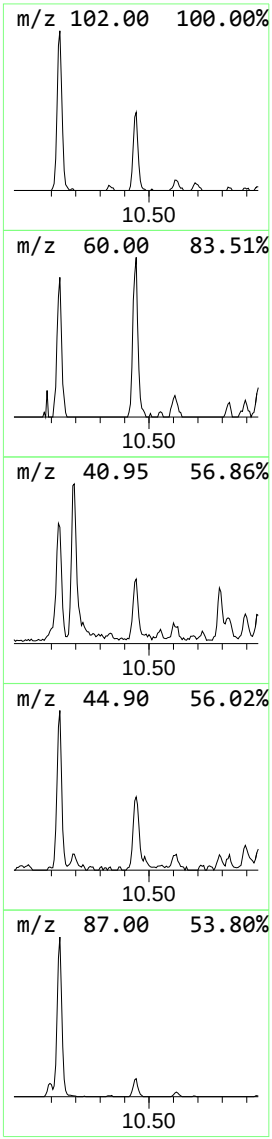
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Thiophene, tetrahydro-3-met... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.447	5.72 ug/l	50213	Chlorobenzene-d5	10.094

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	81
2	Dihydro-3-(2H)-thiophenone	102	C4H6OS	001003-04-9	55
3	2-Thiazolamine, 4,5-dihydro-	102	C3H6N2S	001779-81-3	35
4	Thiophene, tetrahydro-2-methyl-	102	C5H10S	001795-09-1	25
5	2-Acetyl-2,3,5,6-tetrahydro-1,4-...	145	C6H11NOS	1000281-47-3	16





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
Data File : VX021209.D
Acq On : 15 Mar 2021 18:54
Operator : JC/MD
Sample : M1647-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP1-41730:31

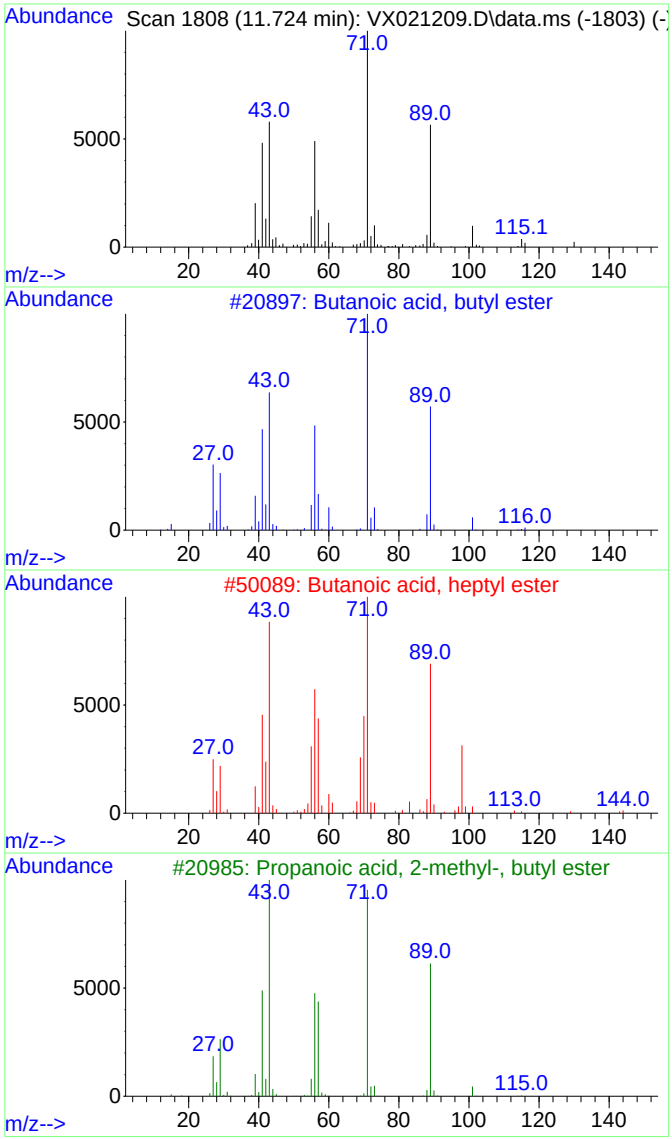
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

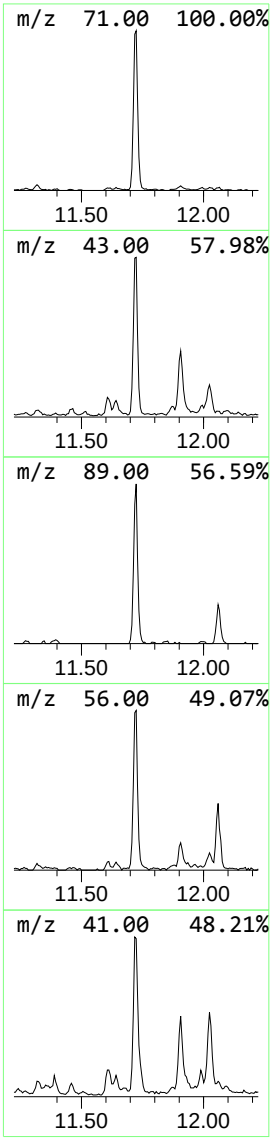
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Butanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.724	12.85 ug/l	107773	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	91
2	Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	72
3	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	72
4	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
5	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	64





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Data File : VX021209.D
Acq On : 15 Mar 2021 18:54
Operator : JC/MD
Sample : M1647-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP1-41730:31

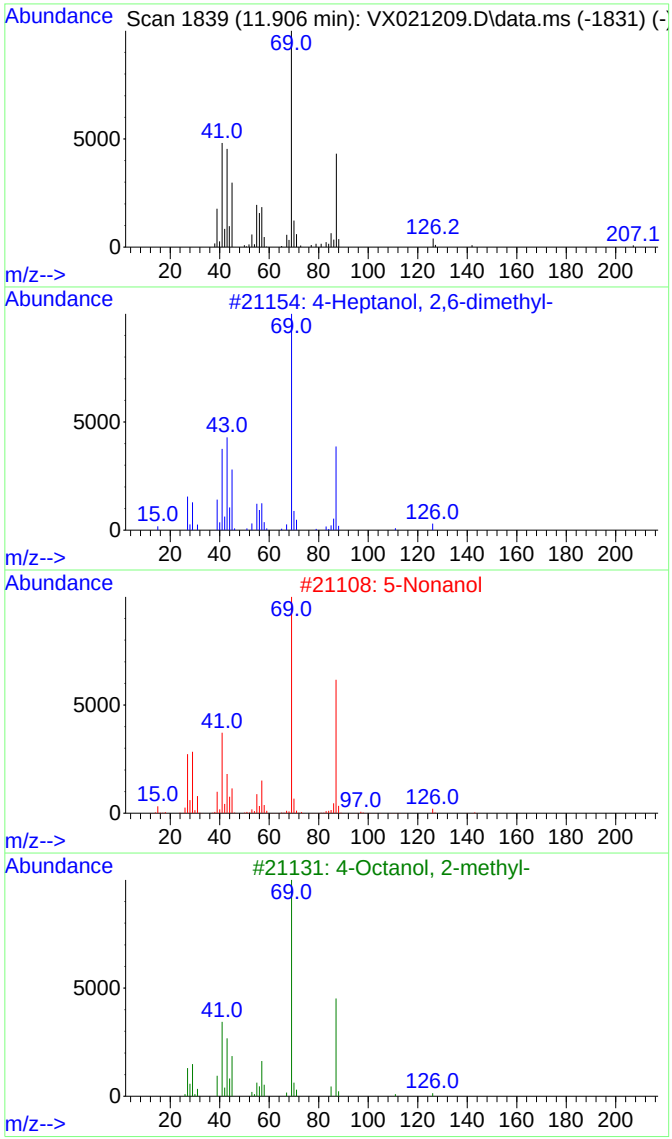
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

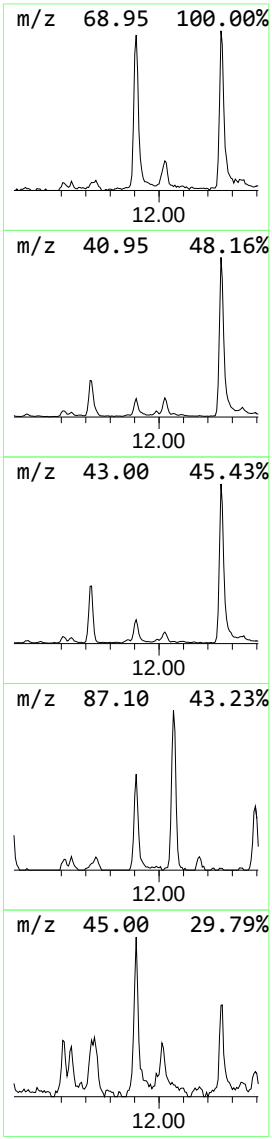
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 4-Heptanol, 2,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.906	6.73 ug/l	56425	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	83
2	5-Nonanol	144	C9H20O	000623-93-8	72
3	4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	72
4	3-Hexanol, 2,5-dimethyl-	130	C8H18O	019550-07-3	64
5	Pentanoic acid, 2-hydroxy-4-meth...	146	C7H14O3	040348-72-9	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
Data File : VX021209.D
Acq On : 15 Mar 2021 18:54
Operator : JC/MD
Sample : M1647-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP1-41730:31

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

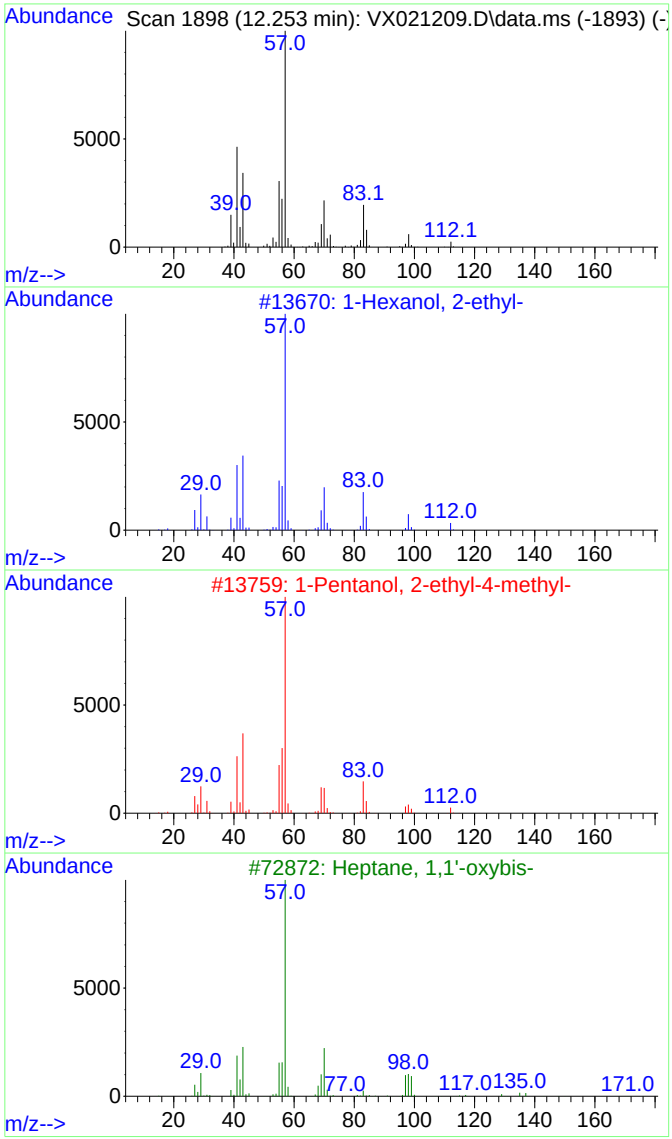
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

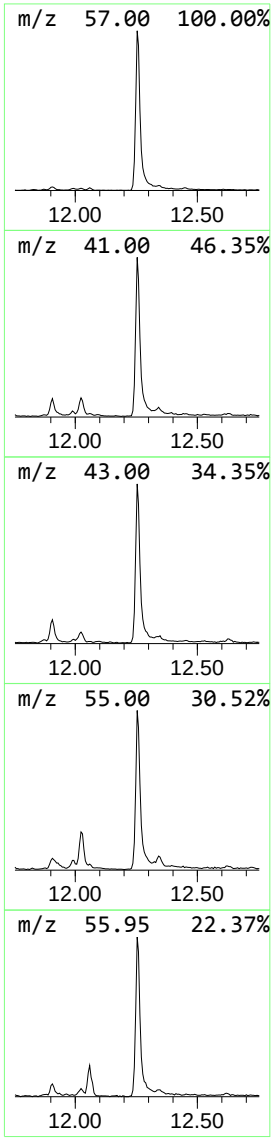
****

Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.253	43.82 ug/l	367539	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5	Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	45





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX031521\
Data File : VX021209.D
Acq On : 15 Mar 2021 18:54
Operator : JC/MD
Sample : M1647-18
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : COMP1-41730:31

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031521W.M
Quant Title : SW846 8260

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown2.099	2.099	9.9	ug/l	46524	1	5.623	235965	50.0
2-Propanethiol,...	3.758	20.2	ug/l	95154	1	5.623	235965	50.0
Butanal	4.299	24.7	ug/l	116364	1	5.623	235965	50.0
Thiophene, tetr...	9.529	21.0	ug/l	184298	3	10.094	439248	50.0
Thiophene, tetr...	10.447	5.7	ug/l	50213	3	10.094	439248	50.0
Butanoic acid, ...	11.724	12.9	ug/l	107773	4	12.059	419355	50.0
4-Heptanol, 2,6...	11.906	6.7	ug/l	56425	4	12.059	419355	50.0
1-Hexanol, 2-et...	12.253	43.8	ug/l	367539	4	12.059	419355	50.0