

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
 Data File : VX028767.D
 Acq On : 17 May 2022 18:52
 Operator : JC/MD
 Sample : N2884-11
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 31804

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\82X051222W.M
 Title : SW846 8260

Signal : TIC: VX028767.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	22	27	42	rBV	159858	383110	21.77%	2.942%
2	1.563	72	78	88	rVB9	15907	36453	2.07%	0.280%
3	2.294	192	198	206	rBV	37151	62881	3.57%	0.483%
4	2.380	206	212	227	rVB	86958	152242	8.65%	1.169%
5	2.526	230	236	246	rBV2	31723	78049	4.43%	0.599%
6	2.959	301	307	317	rVB3	7772	19523	1.11%	0.150%
7	4.233	506	516	529	rBV2	23981	66563	3.78%	0.511%
8	4.562	562	570	581	rVB3	6314	18514	1.05%	0.142%
9	5.391	695	706	721	rBV	215079	623386	35.42%	4.787%
10	5.556	721	733	751	rVB	341498	959947	54.54%	7.371%
11	5.958	788	799	815	rBV	227208	601596	34.18%	4.619%
12	6.111	818	824	834	rVB3	8676	25677	1.46%	0.197%
13	6.763	921	931	945	rBV	553370	1301659	73.95%	9.995%
14	7.214	995	1005	1015	rBV	26088	63748	3.62%	0.489%
15	8.653	1233	1241	1248	rBV	1088946	1760208	100.00%	13.516%
16	8.720	1248	1252	1256	rVV	34411	54152	3.08%	0.416%
17	8.769	1256	1260	1286	rVB5	27265	89471	5.08%	0.687%
18	9.238	1332	1337	1342	rBV2	13464	20937	1.19%	0.161%
19	9.561	1385	1390	1413	rBV	51605	153821	8.74%	1.181%
20	10.055	1465	1471	1482	rBV	1224097	1638751	93.10%	12.583%
21	10.153	1482	1487	1492	rBV	28247	40027	2.27%	0.307%
22	10.506	1540	1545	1553	rVB	28206	36352	2.07%	0.279%
23	10.683	1571	1574	1580	rVB	25117	31981	1.82%	0.246%
24	10.756	1581	1586	1593	rBV2	51479	83170	4.73%	0.639%
25	11.085	1634	1640	1645	rBV	983944	1283152	72.90%	9.853%
26	11.134	1645	1648	1654	rVB	57272	70089	3.98%	0.538%
27	11.573	1715	1720	1723	rBV	36846	46864	2.66%	0.360%
28	11.604	1723	1725	1734	rVV2	30479	48627	2.76%	0.373%
29	11.689	1734	1739	1745	rVB	36983	49231	2.80%	0.378%
30	11.829	1755	1762	1765	rBV3	19372	34525	1.96%	0.265%
31	11.866	1765	1768	1779	rVV	105574	159216	9.05%	1.223%
32	11.957	1779	1783	1789	rVV5	13013	31899	1.81%	0.245%
33	12.024	1789	1794	1802	rVB	1282175	1589167	90.28%	12.203%
34	12.219	1821	1826	1836	rBV	891569	1146584	65.14%	8.804%
35	12.305	1837	1840	1851	rVV6	29229	62918	3.57%	0.483%
36	12.567	1878	1883	1893	rVB4	14627	29821	1.69%	0.229%

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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 >
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Title : SW846 8260

37	13.750	2072	2077	2079	rBV3	15557	22021	1.25%	0.169%
38	13.774	2079	2081	2086	rVV	15112	21131	1.20%	0.162%
39	13.847	2090	2093	2100	rVB	26161	38596	2.19%	0.296%
40	13.914	2100	2104	2109	rBV	23974	35836	2.04%	0.275%
41	14.640	2215	2223	2233	rVB4	13118	33612	1.91%	0.258%
42	15.975	2437	2442	2447	rBV9	9330	17651	1.00%	0.136%

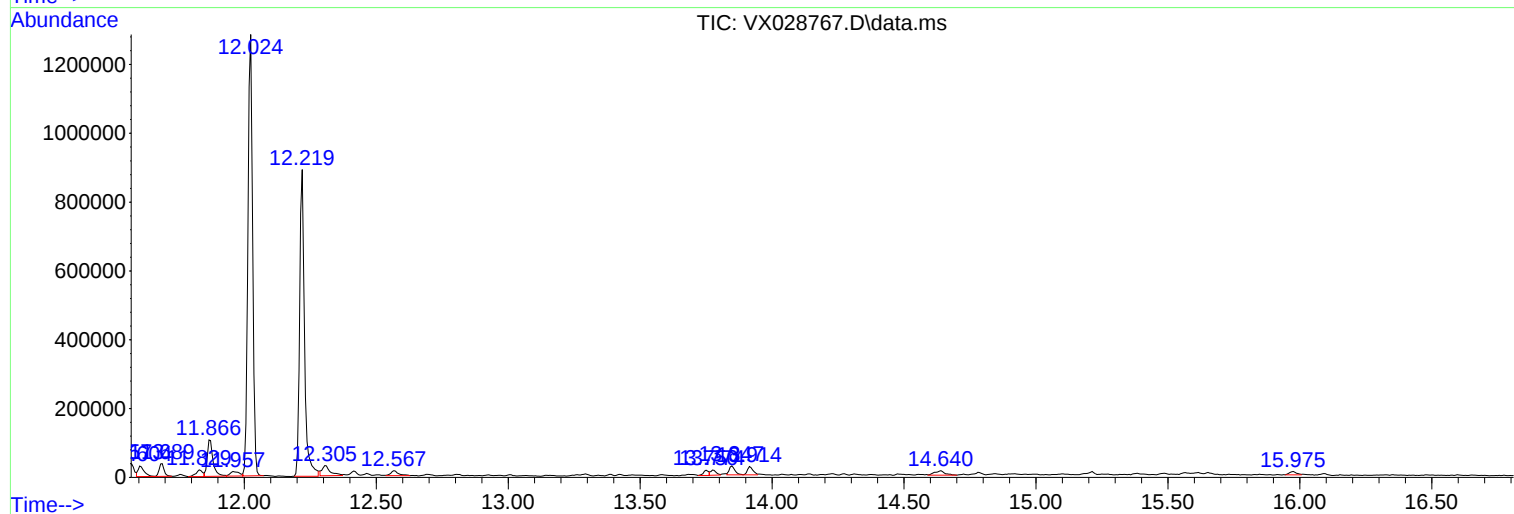
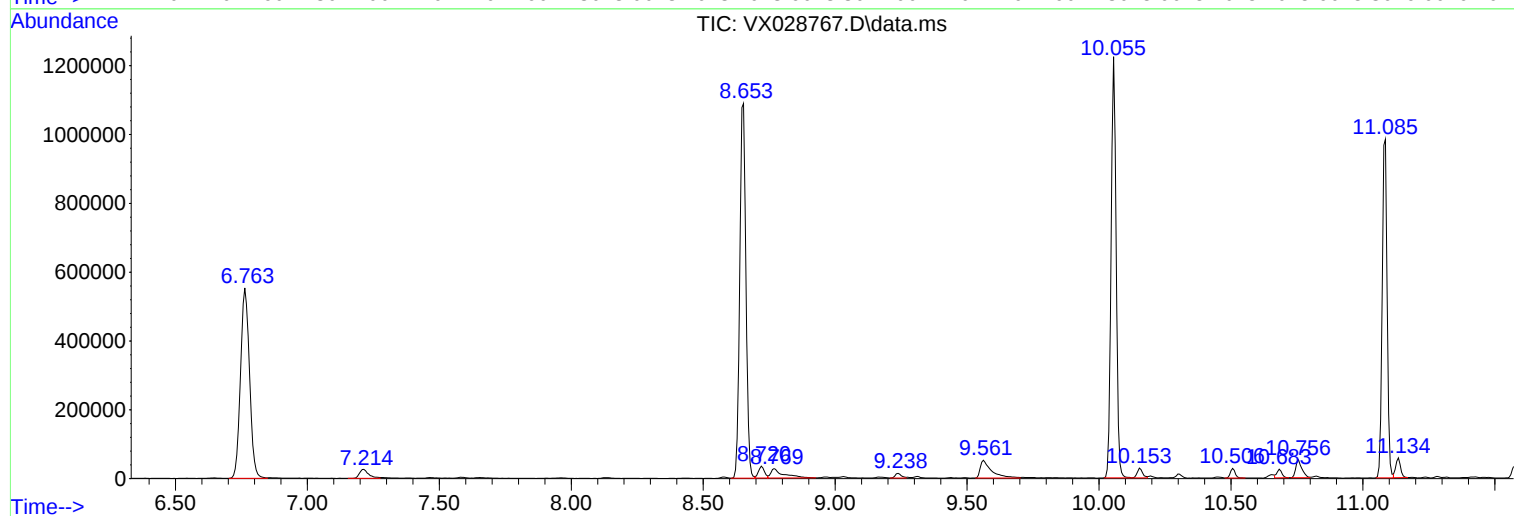
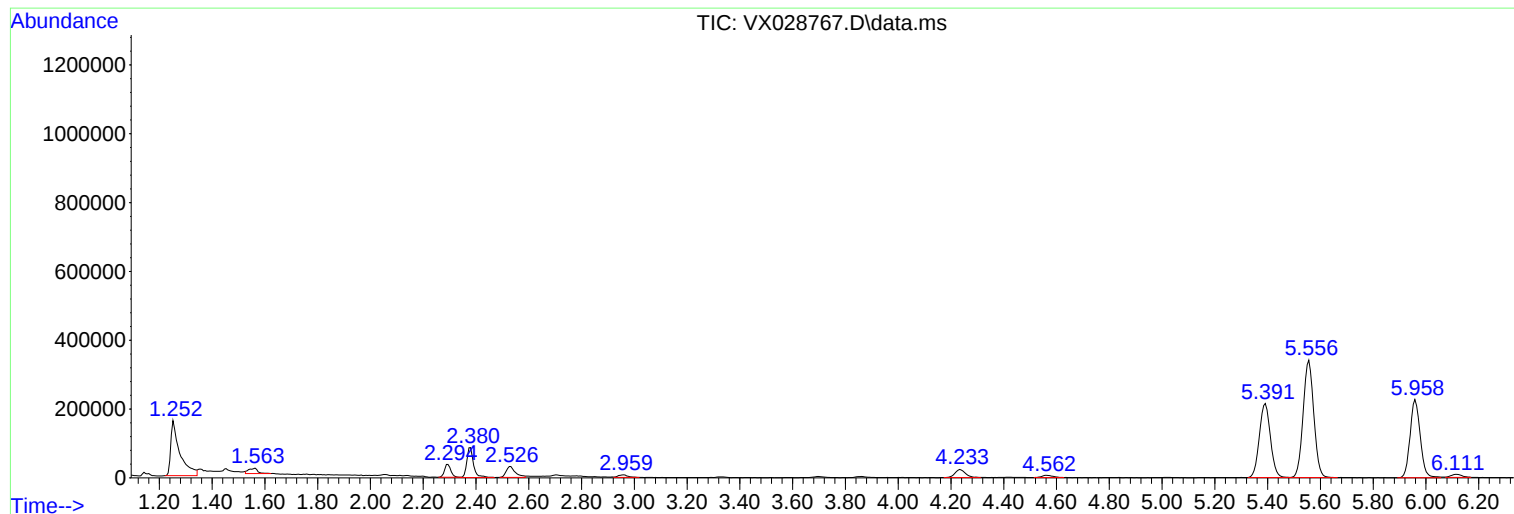
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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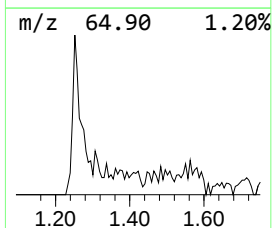
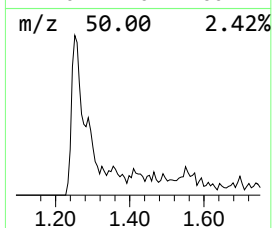
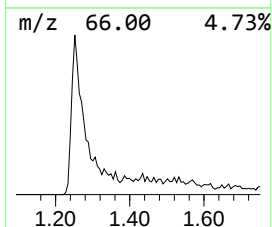
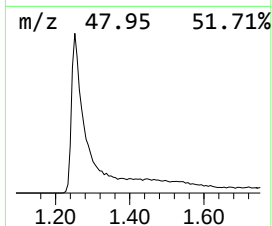
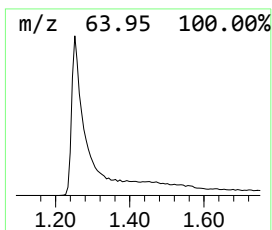
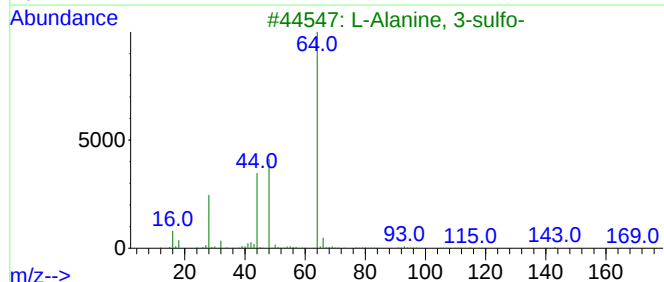
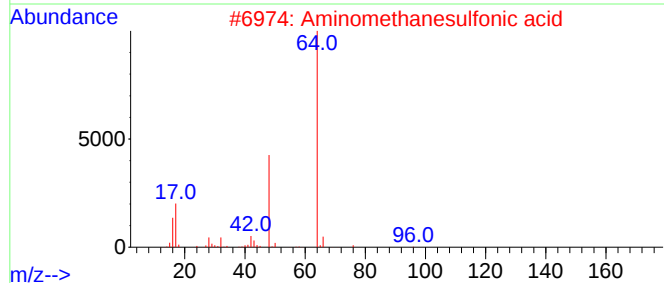
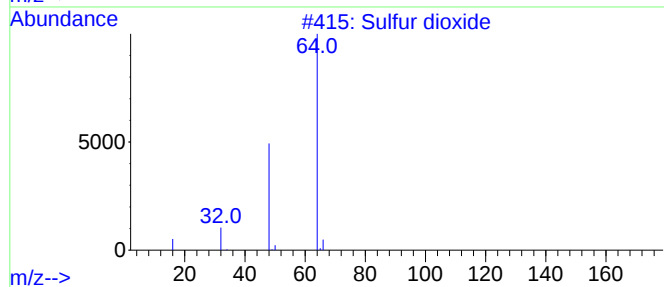
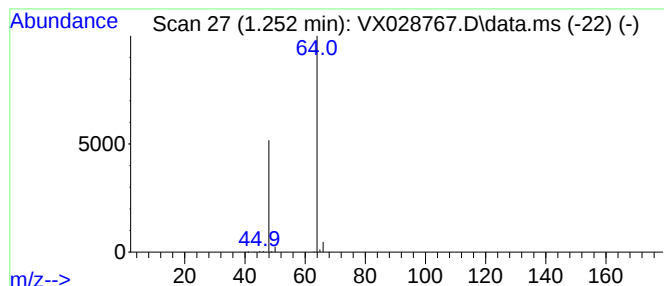
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	19.95 ug/l	383110	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethyl Chloride	64	C2H5Cl	000075-00-3	3
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	3



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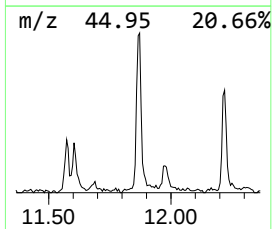
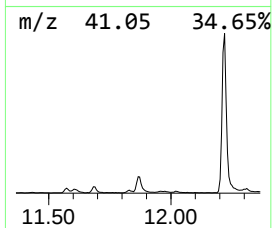
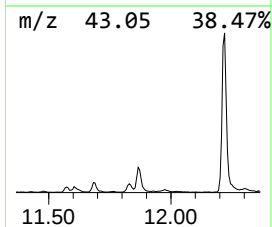
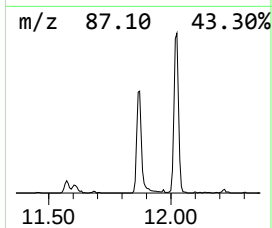
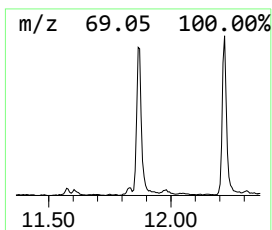
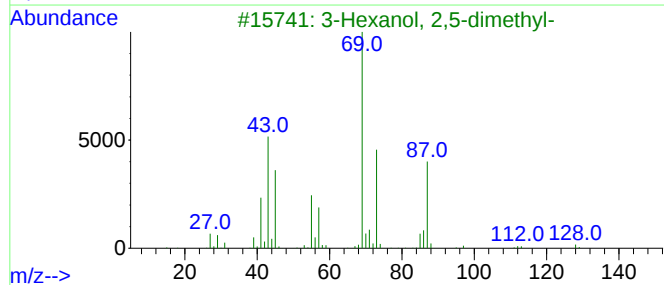
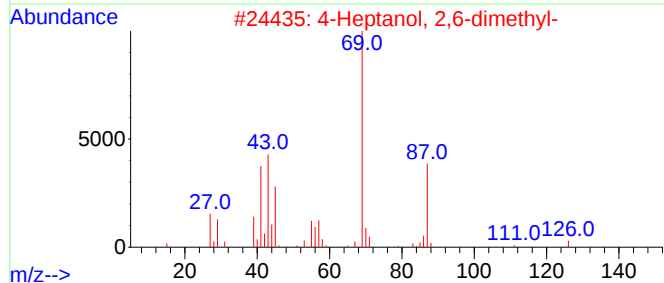
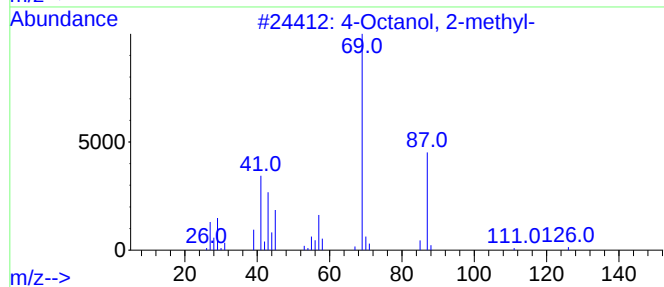
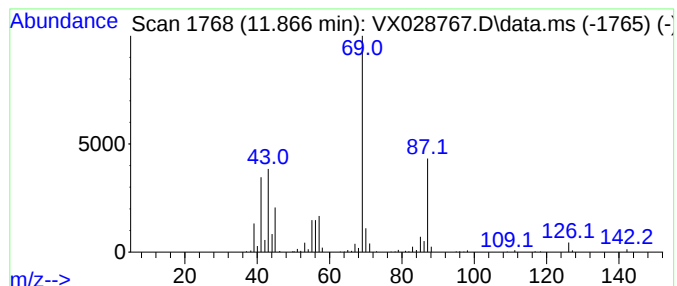
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 4-Octanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.866	5.01 ug/l	159216	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	78
2			4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	74
3			3-Hexanol, 2,5-dimethyl-	130	C8H18O	019550-07-3	72
4			1,2-Hexanediol	118	C6H14O2	006920-22-5	64
5			5-Nonanol	144	C9H20O	000623-93-8	64



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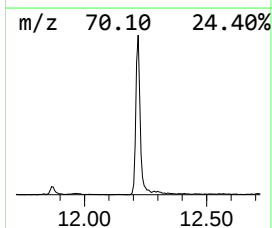
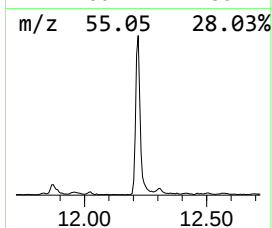
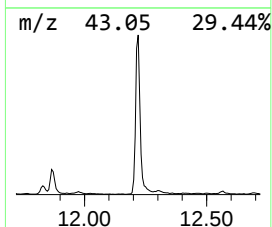
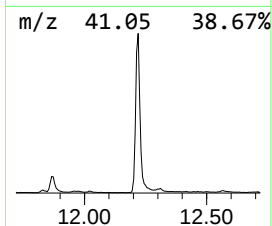
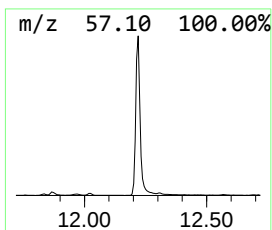
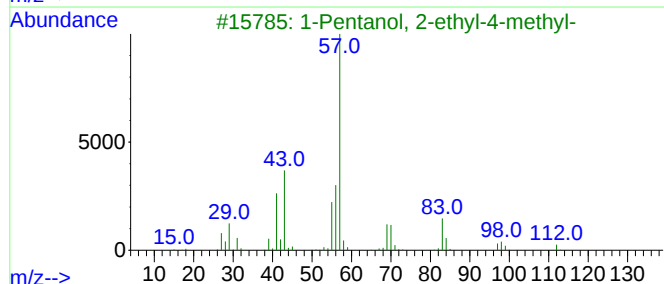
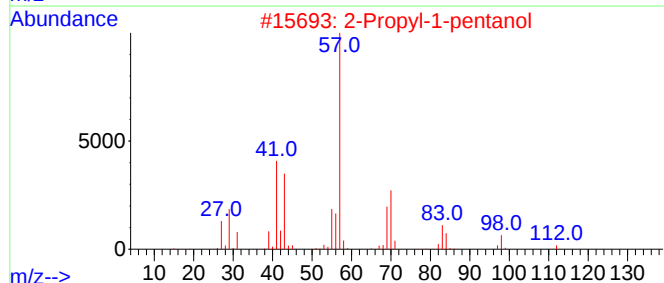
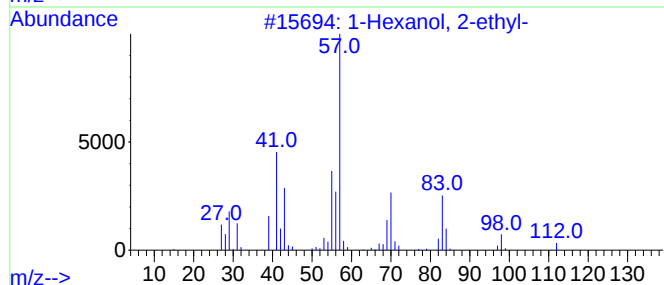
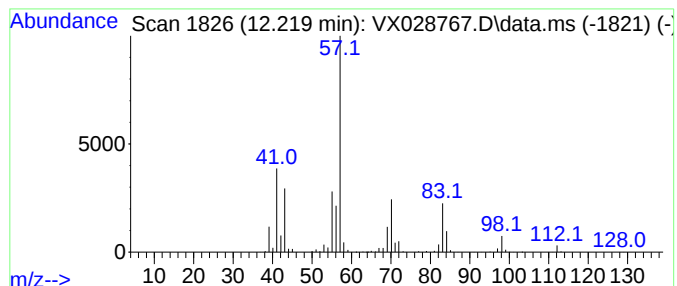
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	36.08 ug/l	1146580	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	59
3			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47



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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.252	19.9	ug/l	383110	1	5.556	959947	50.0
4-Octanol, 2-me...	11.866	5.0	ug/l	159216	4	12.024	1589170	50.0
1-Hexanol, 2-et...	12.219	36.1	ug/l	1146580	4	12.024	1589170	50.0