LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052522\
Data File : VX028983.D
Acq On : 26 May 2022 05:02
Operator : JC/MD
Sample : N3024-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31794

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: VX028983.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	19	rVB	264408	224834	11.56%	1.422%
2	1.252	21	27	43	rBV	206649	490389	25.21%	3.101%
3	1.367	43	46	52	rVB	27452	34251	1.76%	0.217%
4	2.379	206	212	224	rBV	74660	127730	6.57%	0.808%
5	2.526	229	236	243	rBV2	33252	78205	4.02%	0.494%
6	2.959	299	307	322	rBV3	27598	70702	3.63%	0.447%
7	3.696	417	428	445	rBV	77996	219555	11.29%	1.388%
8	4.233	503	516	530	rBV2	78519	232002	11.93%	1.467%
9	4.568	562	571	581	rVB	7086	19480	1.00%	0.123%
10	5.391	694	706	722	rBV2	226700	668718	34.38%	4.228%
11	5.556	722	733	749	rVB	363766	1028399	52.87%	6.503%
12	5.958	789	799	807	rBV	235321	616888	31.72%	3.901%
13	6.043	807	813	833	rVB	67773	196153	10.08%	1.240%
14	6.763	920	931	946	rBV	587355	1387032	71.31%	8.770%
15	7.683	1074	1082	1090	rVB5	9097	23731	1.22%	0.150%
16	8.653	1233	1241	1248	rBV	1188065	1891758	97.26%	11.962%
17	8.720	1248	1252	1257	rVV	94421	144565	7.43%	0.914%
18	9.494	1374	1379	1386	rVB	17493	27580	1.42%	0.174%
19	10.055	1465	1471	1482	rBV	1297882	1736134	89.26%	10.978%
20	10.159	1483	1488	1491	rVV	17640	28511	1.47%	0.180%
21	10.195	1491	1494	1501	rVV	19089	28021	1.44%	0.177%
22	10.305	1501	1512	1520	rVB	75436	113632	5.84%	0.718%
23	10.506	1541	1545	1552	rBV	33436	44784	2.30%	0.283%
24	10.646	1562	1568	1572	rBV	36948	54687	2.81%	0.346%
25	10.756	1581	1586	1599	rBV	91819	139647	7.18%	0.883%
26	11.085	1634	1640	1645	rBV	1040182	1362372	70.04%	8.614%
27	11.134	1645	1648	1655	rVB	71992	90928	4.67%	0.575%
28	11.573	1715	1720	1723	rBV	71466	96536	4.96%	0.610%
29	11.603	1723	1725	1731	rVB2	46938	65208	3.35%	0.412%
30	11.756	1745	1750	1755	rVV	21328	27988	1.44%	0.177%
31	11.829	1755	1762	1765	rVV3	27951	48551	2.50%	0.307%
32	11.872	1765	1769	1781	rVV	170059	273013	14.04%	1.726%
33	11.975	1781	1786	1789	rVV5	13238	25111	1.29%	0.159%
34	12.024	1789	1794	1801	rVB	1389405	1706534	87.74%	10.790%
35	12.219	1821	1826	1837	rBV	1535722	1945060	100.00%	12.299%
36	12.305	1837	1840	1847	rVB4	42247	69505	3.57%	0.439%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052522\
Data File : VX028983.D
Acq On : 26 May 2022 05:02
Operator : JC/MD
Sample : N3024-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31794

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

37	12.567	1879	1883	1888	rBV4	13237	19961	1.03%	0.126%
38	12.963	1945	1948	1952	rVB	16072	21023	1.08%	0.133%
39	13.292	1998	2002	2008	rVB2	15239	20964	1.08%	0.133%
40	13.749	2074	2077	2079	rVV2	21687	28779	1.48%	0.182%
41	13.780	2079	2082	2086	rVV	50654	66143	3.40%	0.418%
42	13.847	2088	2093	2100	rVV	69390	104557	5.38%	0.661%
43	13.914	2100	2104	2118	rVB	86063	141259	7.26%	0.893%
44	14.639	2216	2223	2227	rBV	34274	51347	2.64%	0.325%
45	14.780	2242	2246	2250	rBV	17708	22957	1.18%	0.145%

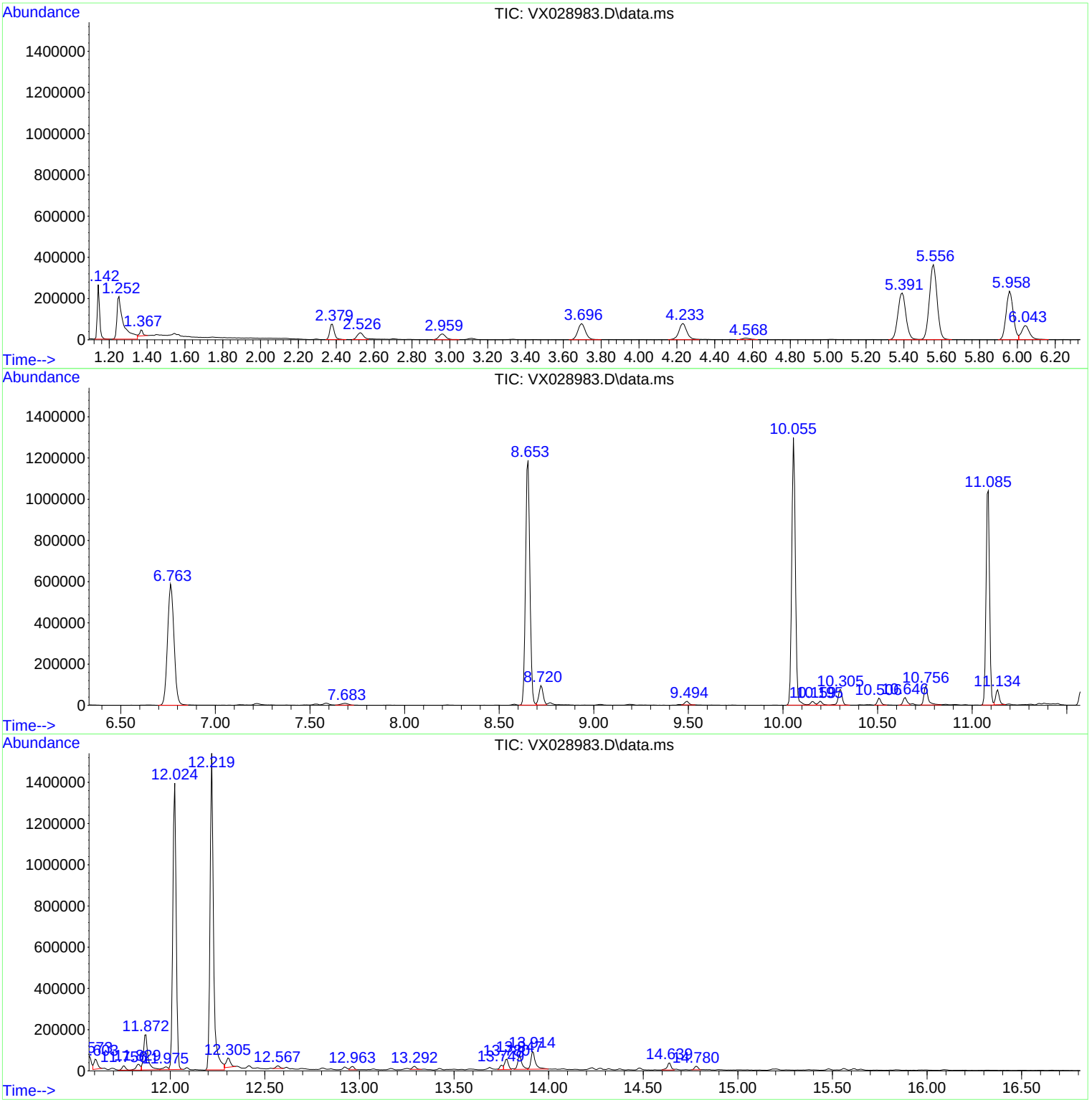
Sum of corrected areas: 15815184

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052522\
Data File : VX028983.D
Acq On : 26 May 2022 05:02
Operator : JC/MD
Sample : N3024-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31794

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052522\
Data File : VX028983.D
Acq On : 26 May 2022 05:02
Operator : JC/MD
Sample : N3024-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31794

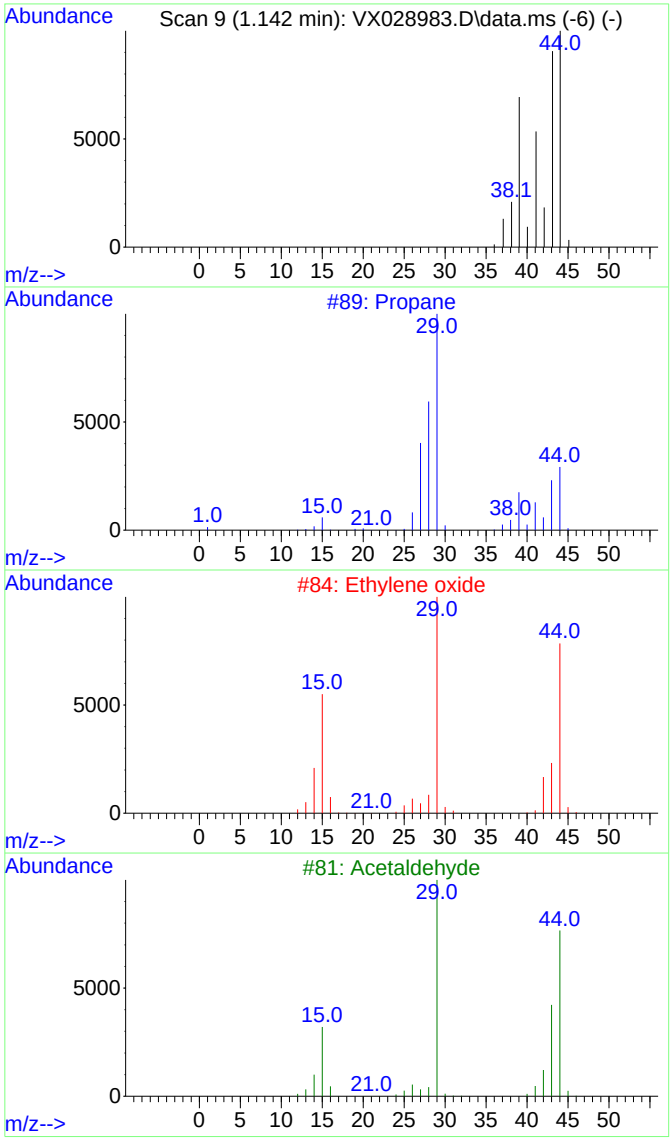
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

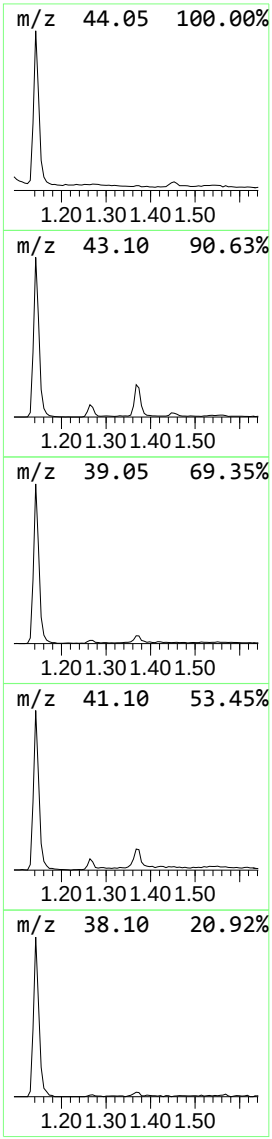
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	10.93 ug/l	224834	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	83
2	Ethylene oxide	44	C2H4O	000075-21-8	5
3	Acetaldehyde	44	C2H4O	000075-07-0	5
4	Propene	42	C3H6	000115-07-1	4
5	Ethyne, fluoro-	44	C2HF	002713-09-9	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052522\
Data File : VX028983.D
Acq On : 26 May 2022 05:02
Operator : JC/MD
Sample : N3024-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31794

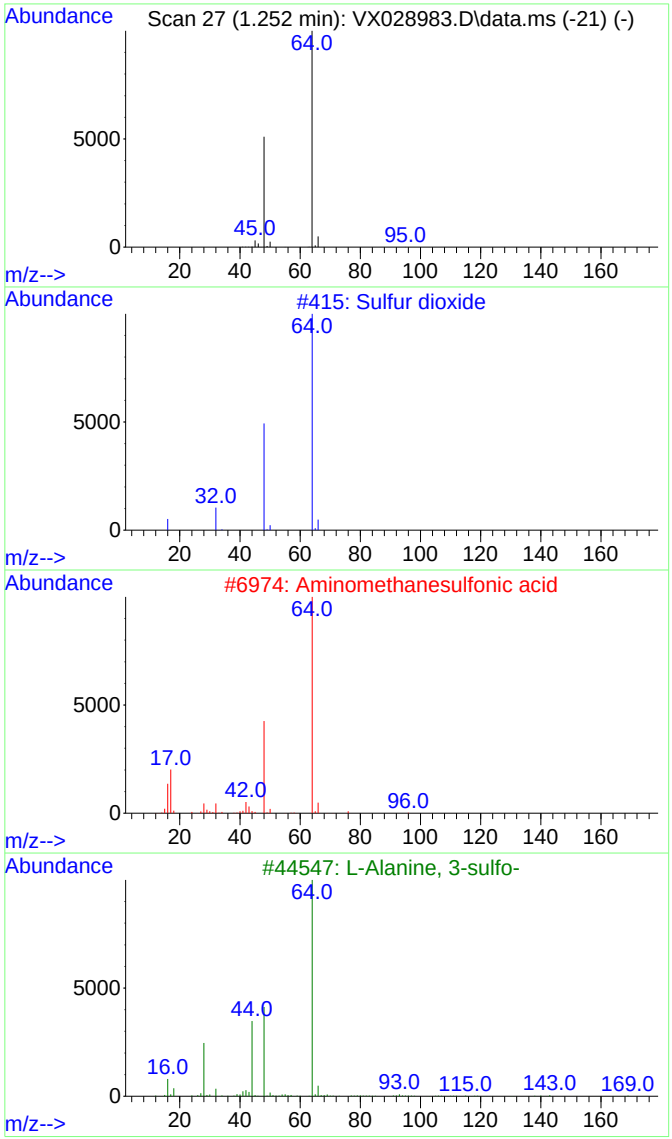
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

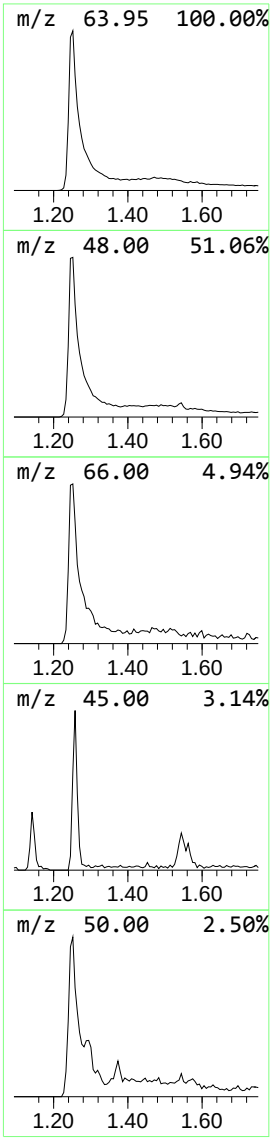
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	23.84 ug/l	490389	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	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052522\
Data File : VX028983.D
Acq On : 26 May 2022 05:02
Operator : JC/MD
Sample : N3024-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31794

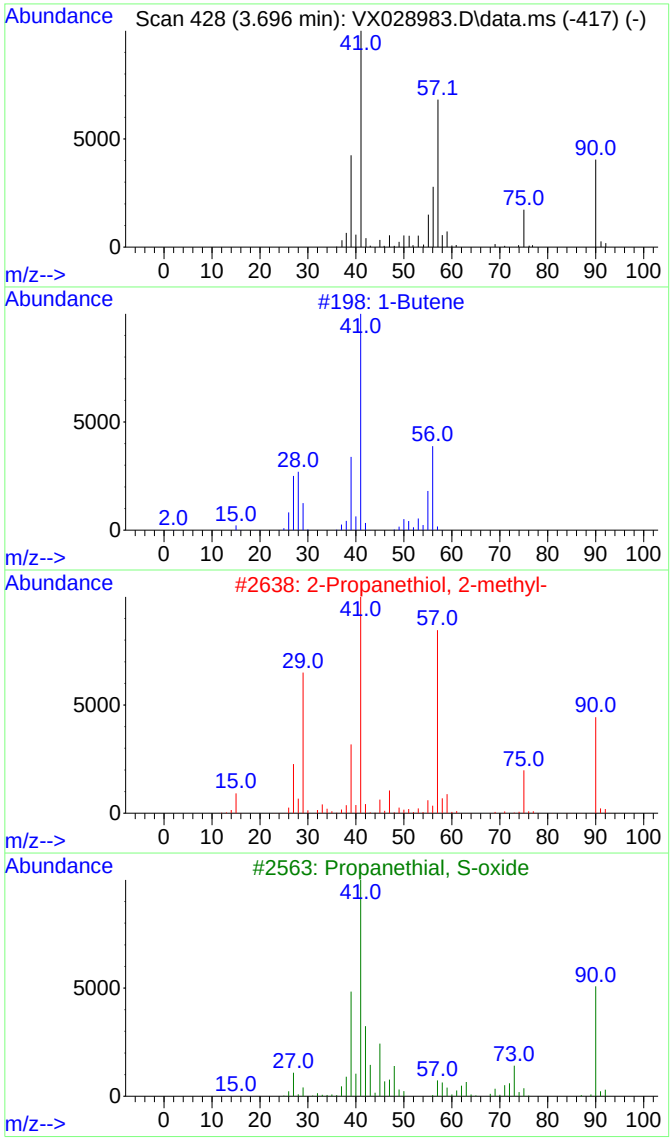
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

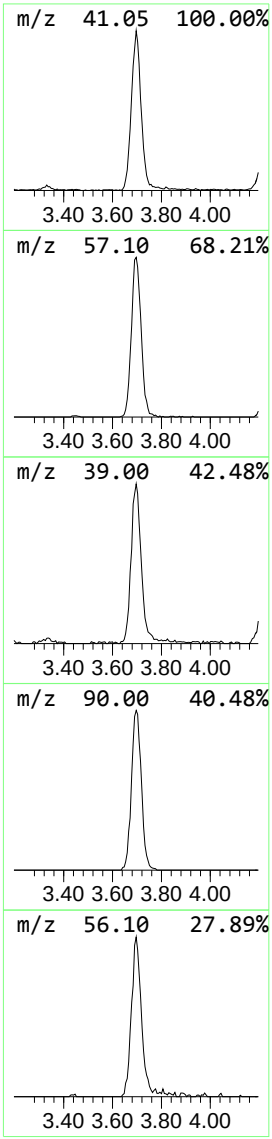
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 unknown3.696 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.696	10.67 ug/l	219555	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butene	56	C4H8	000106-98-9	46
2	2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	46
3	Propanethial, S-oxide	90	C3H6OS	032157-29-2	42
4	Propane, 2-methyl-1-nitro-	103	C4H9NO2	000625-74-1	37
5	2-Butanethiol	90	C4H10S	000513-53-1	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052522\
Data File : VX028983.D
Acq On : 26 May 2022 05:02
Operator : JC/MD
Sample : N3024-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31794

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

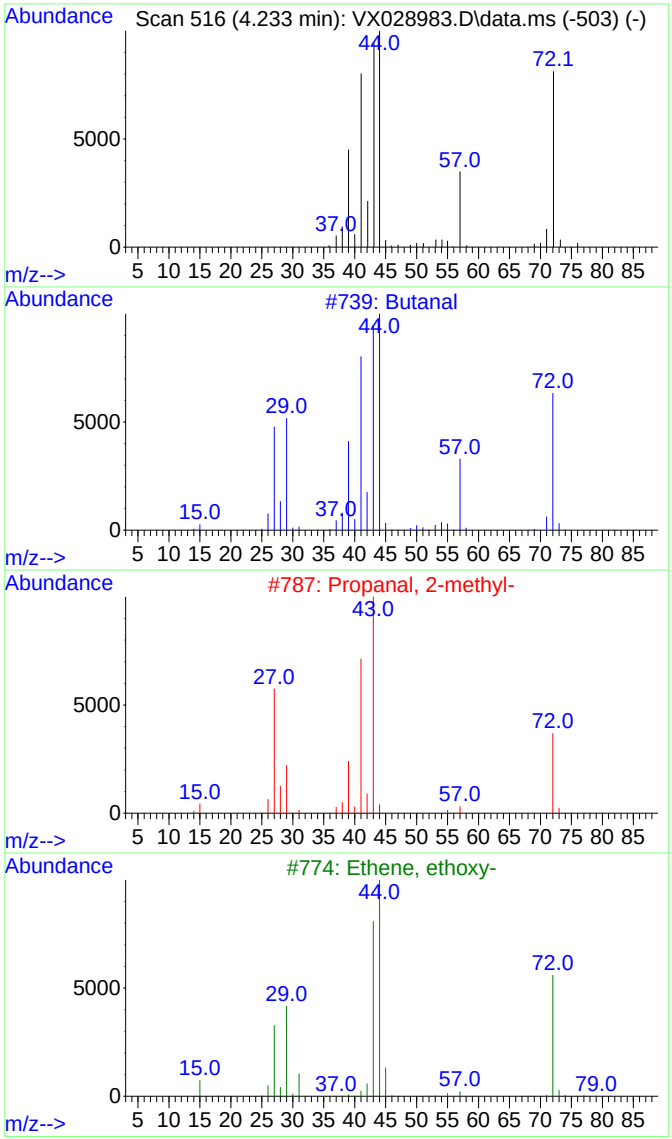
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

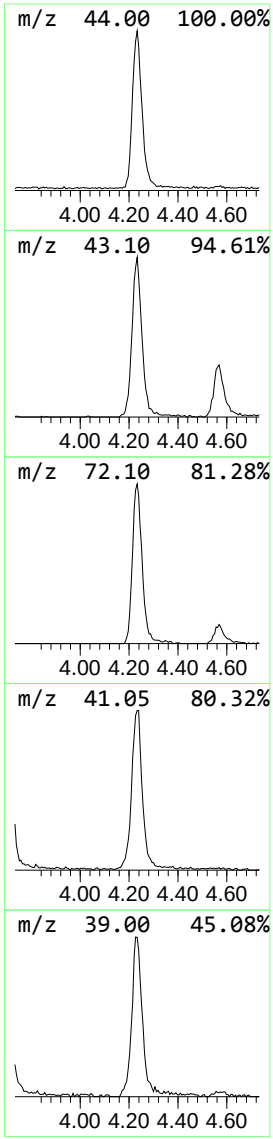
****

Peak Number 4 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.233	11.28 ug/l	232002	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3	Ethene, ethoxy-	72	C4H8O	000109-92-2	40
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38
5	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052522\
Data File : VX028983.D
Acq On : 26 May 2022 05:02
Operator : JC/MD
Sample : N3024-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31794

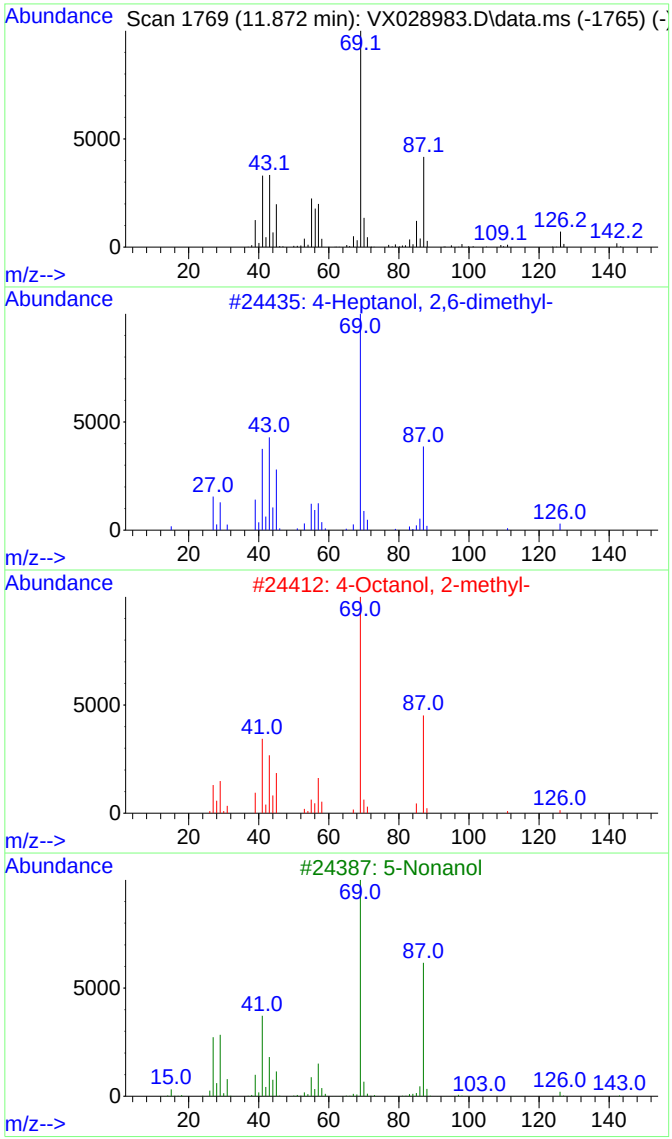
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

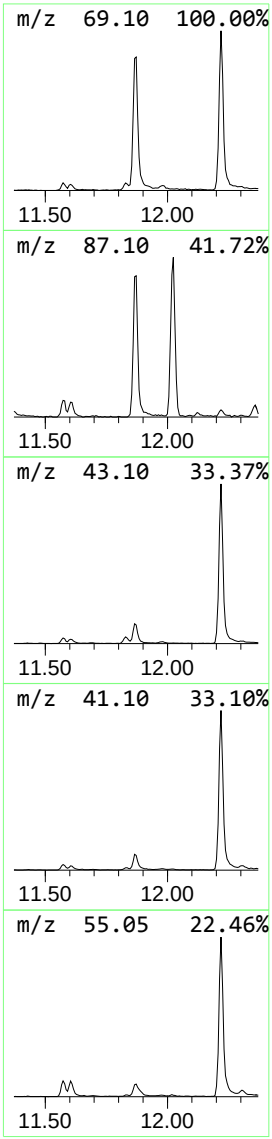
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4-Heptanol, 2,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.872	8.00 ug/l	273013	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	78
2	4-Octanol, 2-methyl-	144	C9H20O	040575-41-5	72
3	5-Nonanol	144	C9H20O	000623-93-8	64
4	3-Heptanol, 2-methyl-	130	C8H18O	018720-62-2	59
5	2-Butenoic acid, butyl ester	142	C8H14O2	007299-91-4	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052522\
Data File : VX028983.D
Acq On : 26 May 2022 05:02
Operator : JC/MD
Sample : N3024-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31794

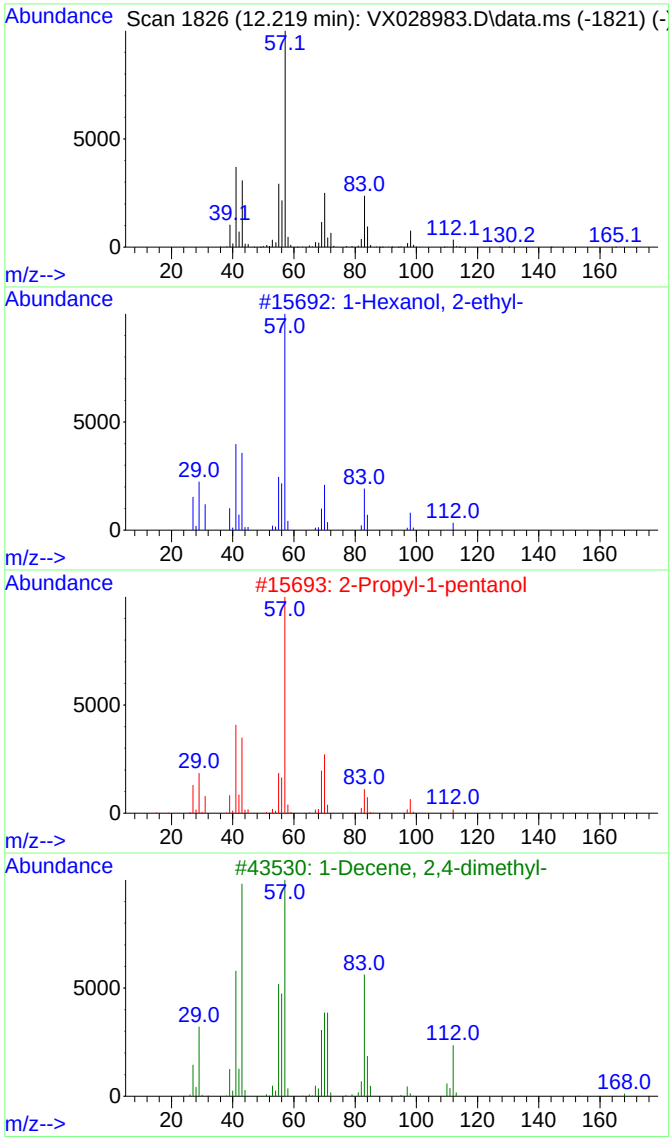
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

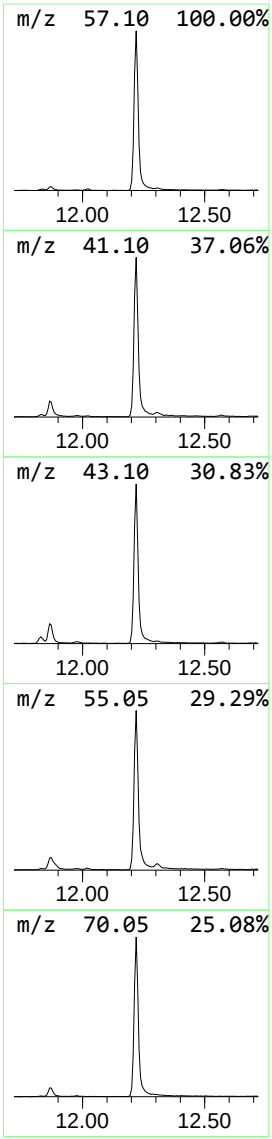
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	56.99 ug/l	1945060	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-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	50
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5	2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	053800-08-1	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052522\
Data File : VX028983.D
Acq On : 26 May 2022 05:02
Operator : JC/MD
Sample : N3024-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 50 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31794

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane	1.142	10.9	ug/l	224834	1	5.556	1028400	50.0
Sulfur dioxide	1.252	23.8	ug/l	490389	1	5.556	1028400	50.0
unknown3.696	3.696	10.7	ug/l	219555	1	5.556	1028400	50.0
Butanal	4.233	11.3	ug/l	232002	1	5.556	1028400	50.0
4-Heptanol, 2,6...	11.872	8.0	ug/l	273013	4	12.024	1706530	50.0
1-Hexanol, 2-et...	12.219	57.0	ug/l	1945060	4	12.024	1706530	50.0