LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042224\
Data File : VX041201.D
Acq On : 22 Apr 2024 19:38
Operator : JC/MD
Sample : P2186-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-2030

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\82X042224W.M
Title : SW846 8260

Signal : TIC: VX041201.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	21	25	32	rBV	59275	82981	8.57%	1.205%
2	1.355	41	44	49	rBV	70684	97218	10.04%	1.411%
3	1.746	106	108	115	rBV5	12755	33571	3.47%	0.487%
4	2.398	209	215	227	rBV	16344	38088	3.93%	0.553%
5	3.690	418	427	440	rBV2	23062	65368	6.75%	0.949%
6	5.385	693	705	720	rBV	119155	350870	36.24%	5.094%
7	5.550	721	732	749	rVV	202309	576896	59.59%	8.376%
8	5.952	789	798	818	rBV	115517	309932	32.01%	4.500%
9	6.757	921	930	954	rBV	292117	717564	74.12%	10.418%
10	8.647	1234	1240	1256	rBV	607531	968108	100.00%	14.056%
11	10.055	1465	1471	1491	rBV	597045	856524	88.47%	12.436%
12	10.640	1563	1567	1573	rBV	6915	10342	1.07%	0.150%
13	11.079	1634	1639	1652	rBV	532597	709616	73.30%	10.303%
14	11.689	1733	1739	1743	rBV2	7373	11832	1.22%	0.172%
15	11.756	1744	1750	1762	rVB4	7933	14769	1.53%	0.214%
16	12.024	1788	1794	1801	rVV	660105	840753	86.84%	12.207%
17	12.219	1822	1826	1829	rBV2	8790	14369	1.48%	0.209%
18	13.292	1992	2002	2007	rBV2	9337	16039	1.66%	0.233%
19	13.591	2046	2051	2061	rBV	177072	274156	28.32%	3.980%
20	13.749	2073	2077	2087	rVB2	13529	30766	3.18%	0.447%
21	14.073	2127	2130	2134	rVV2	8505	10441	1.08%	0.152%
22	14.225	2150	2155	2162	rVB2	28152	50343	5.20%	0.731%
23	14.323	2167	2171	2176	rBV4	7982	11327	1.17%	0.164%
24	14.371	2176	2179	2183	rBV	16660	19421	2.01%	0.282%
25	14.481	2192	2197	2202	rBV2	32379	46381	4.79%	0.673%
26	14.615	2214	2219	2221	rBV3	27659	37684	3.89%	0.547%
27	14.670	2226	2228	2233	rVB2	16862	21080	2.18%	0.306%
28	14.725	2233	2237	2239	rBV5	8832	12395	1.28%	0.180%
29	14.755	2239	2242	2245	rVV	28500	33455	3.46%	0.486%
30	14.816	2249	2252	2255	rVV2	13778	22485	2.32%	0.326%
31	14.847	2255	2257	2261	rVV3	13003	13627	1.41%	0.198%
32	14.902	2263	2266	2273	rVB2	15952	27521	2.84%	0.400%
33	15.048	2284	2290	2294	rBV2	8121	14408	1.49%	0.209%
34	15.103	2294	2299	2302	rBV4	7531	12973	1.34%	0.188%
35	15.182	2308	2312	2314	rBV	58380	78376	8.10%	1.138%
36	15.274	2320	2327	2331	rVB6	10723	25618	2.65%	0.372%

LSC Area Percent Report

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ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-2030

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\82X042224W.M
Title : SW846 8260

37	15.371	2339	2343	2351	rBV4	17782	32220	3.33%	0.468%
38	15.487	2356	2362	2366	rBV2	67194	113725	11.75%	1.651%
39	15.609	2378	2382	2386	rBV2	34930	58184	6.01%	0.845%
40	15.652	2386	2389	2396	rVB2	22044	43126	4.45%	0.626%
41	15.841	2416	2420	2424	rBV3	13459	22403	2.31%	0.325%
42	15.987	2440	2444	2447	rBV5	8205	11314	1.17%	0.164%
43	16.023	2447	2450	2455	rVB5	11498	19808	2.05%	0.288%
44	16.084	2455	2460	2469	rBV	21438	48939	5.06%	0.711%
45	16.371	2501	2507	2513	rBV2	22713	42341	4.37%	0.615%
46	16.590	2541	2543	2550	rVB3	8169	12823	1.32%	0.186%
47	16.657	2550	2554	2559	rVV2	7533	14471	1.49%	0.210%
48	16.712	2560	2563	2569	rVB5	6274	11056	1.14%	0.161%

Sum of corrected areas: 6887707

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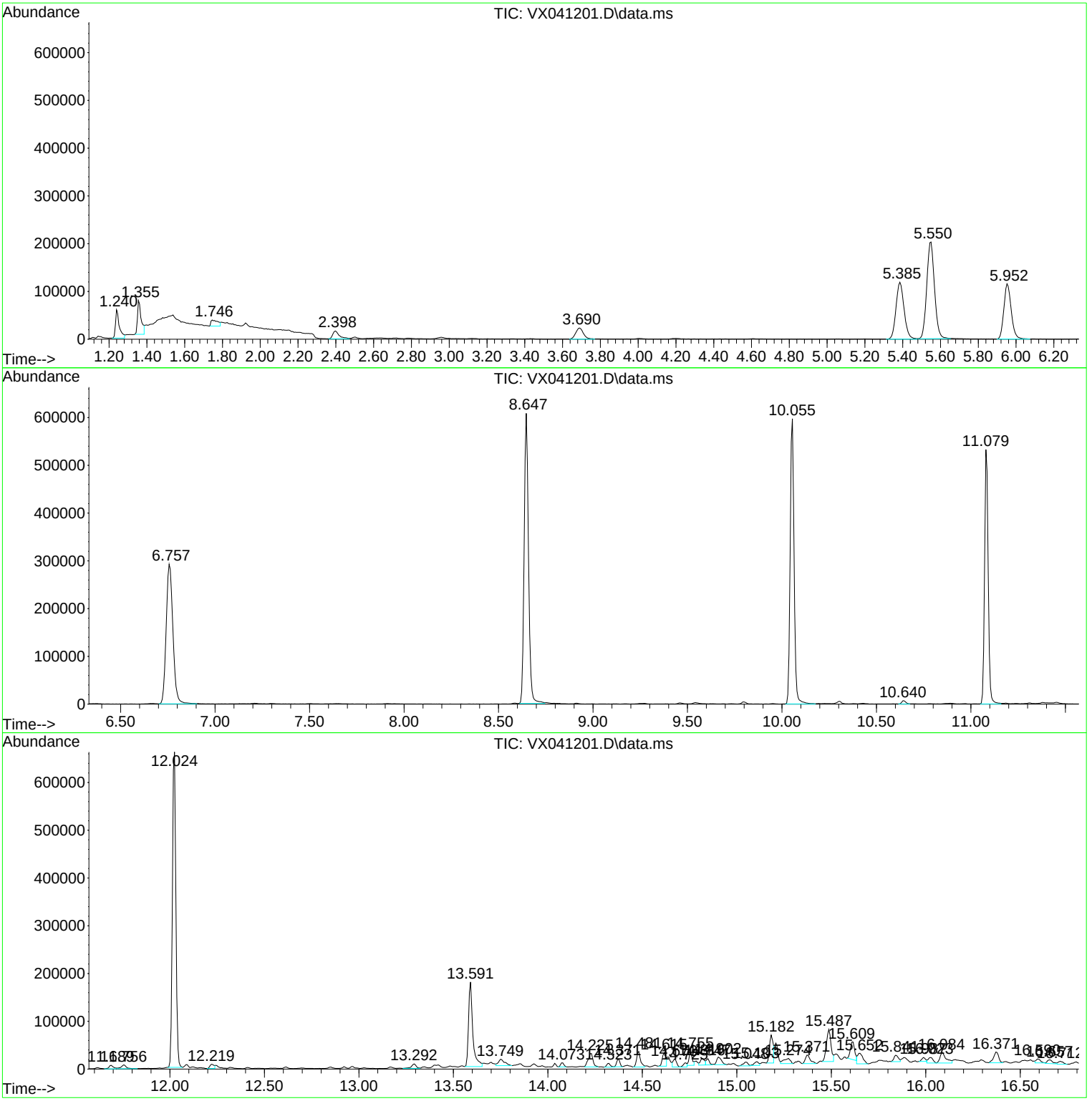
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-2030

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

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



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Data File : VX041201.D
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ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-2030

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

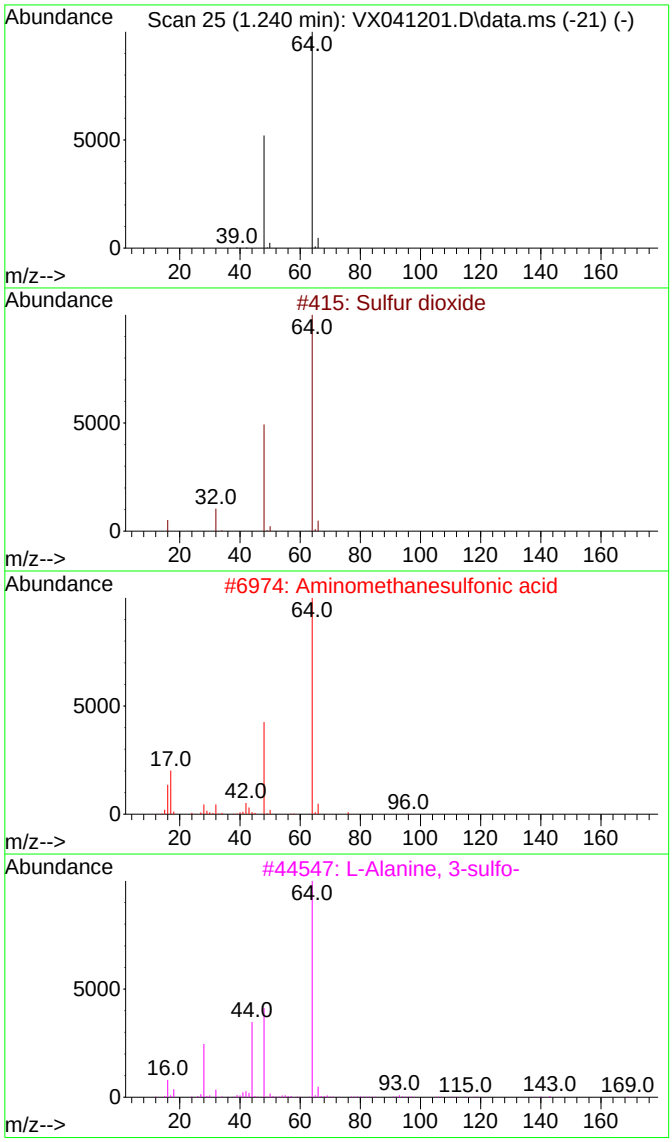
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

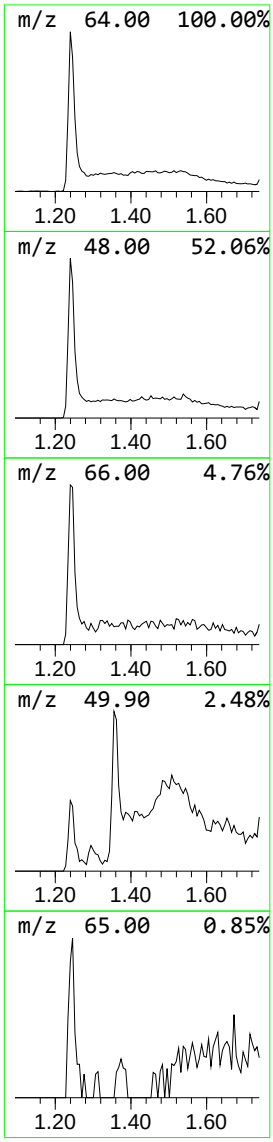
****

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	7.19 ug/l	82981	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





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ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-2030

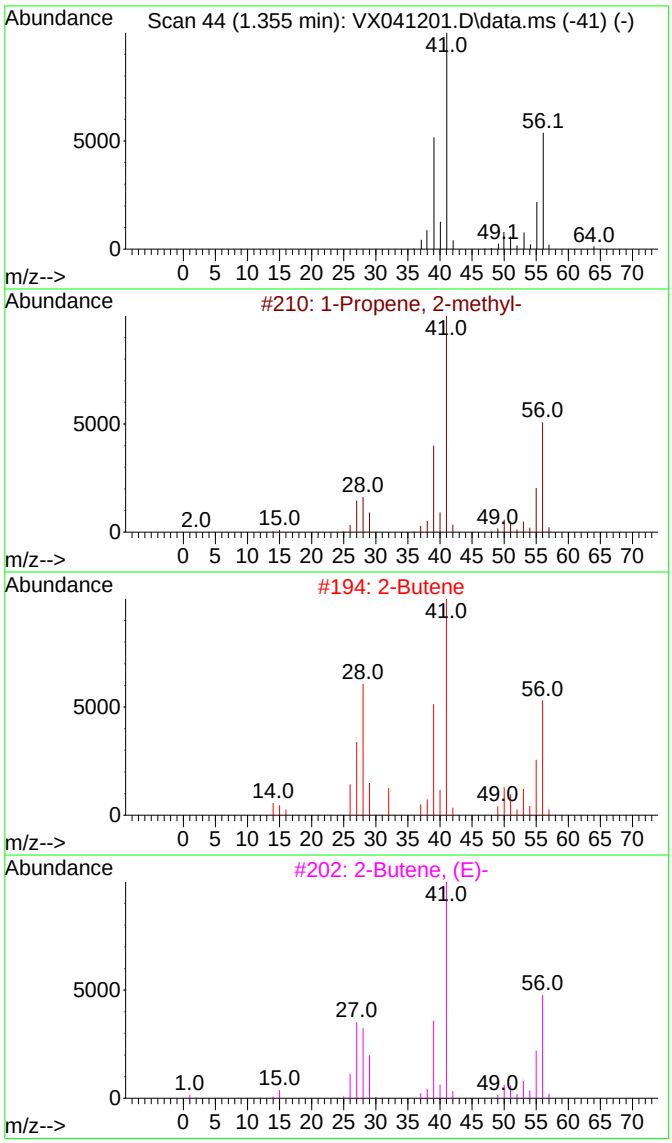
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

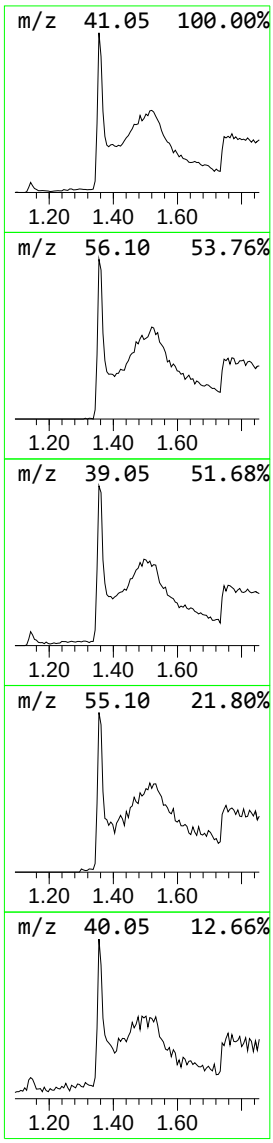
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Propene, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.355	8.43 ug/l	97218	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-	56	C4H8	000115-11-7	90
2	2-Butene	56	C4H8	000107-01-7	80
3	2-Butene, (E)-	56	C4H8	000624-64-6	80
4	Cyclobutane	56	C4H8	000287-23-0	52
5	1-Butene	56	C4H8	000106-98-9	52





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ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-2030

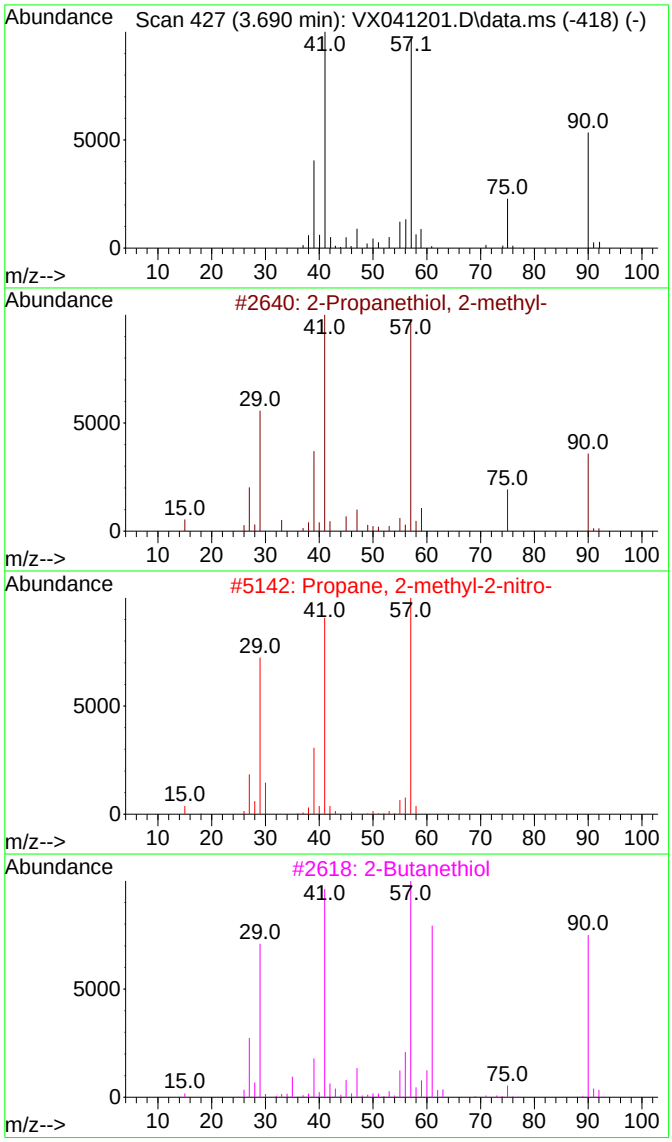
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

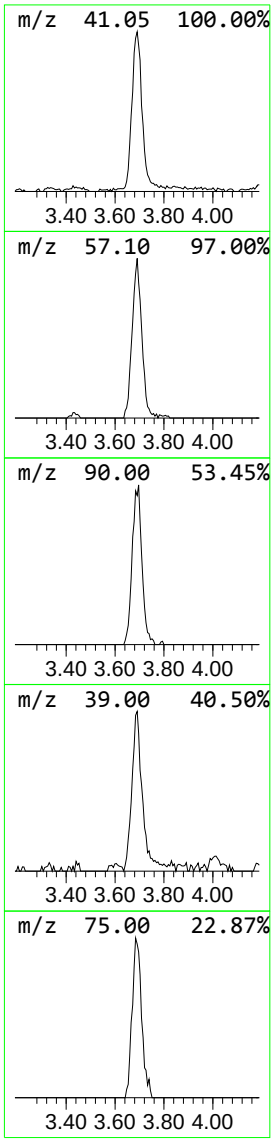
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanethiol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.690	5.67 ug/l	65368	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	70
2	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	43
3	2-Butanethiol	90	C4H10S	000513-53-1	35
4	Propanethial, S-oxide	90	C3H6OS	032157-29-2	33
5	Ethynyl tert-butyl sulfoxide	130	C6H10OS	041463-34-7	22





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Sample : P2186-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-2030

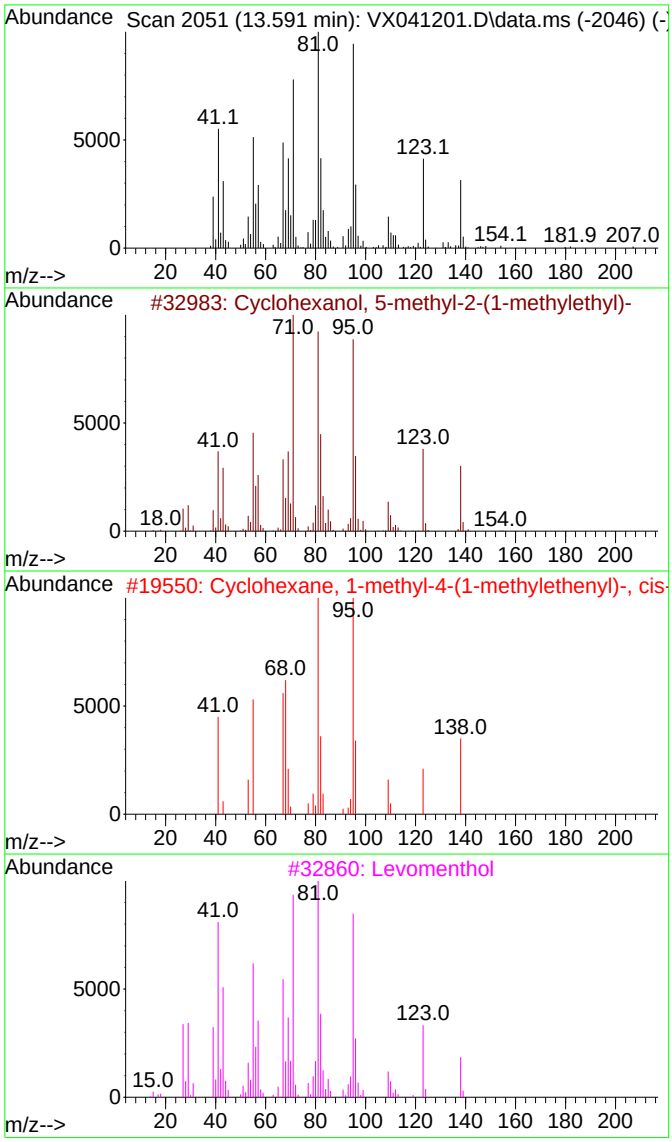
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

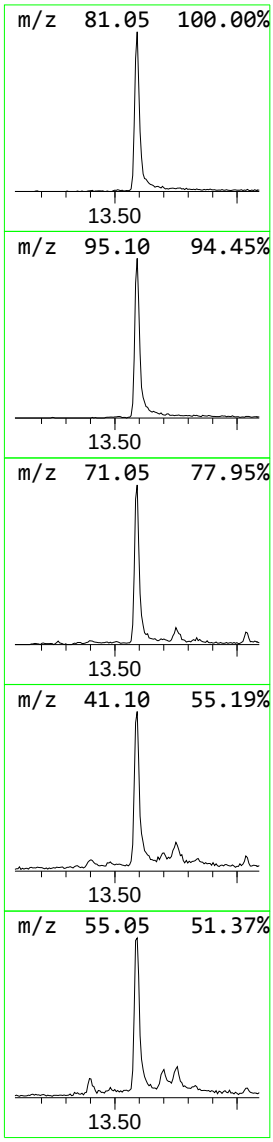
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclohexanol, 5-methyl-2-(1... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.591	16.30 ug/l	274156	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	001490-04-6	90
2	Cyclohexane, 1-methyl-4-(1-methy...	138	C10H18	001879-07-8	86
3	Levomenthol	156	C10H20O	002216-51-5	86
4	dl-Menthol	156	C10H20O	000089-78-1	74
5	d-Menthol	156	C10H20O	015356-60-2	64





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Operator : JC/MD
Sample : P2186-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NWB-2030

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.M
Quant Title : SW846 8260

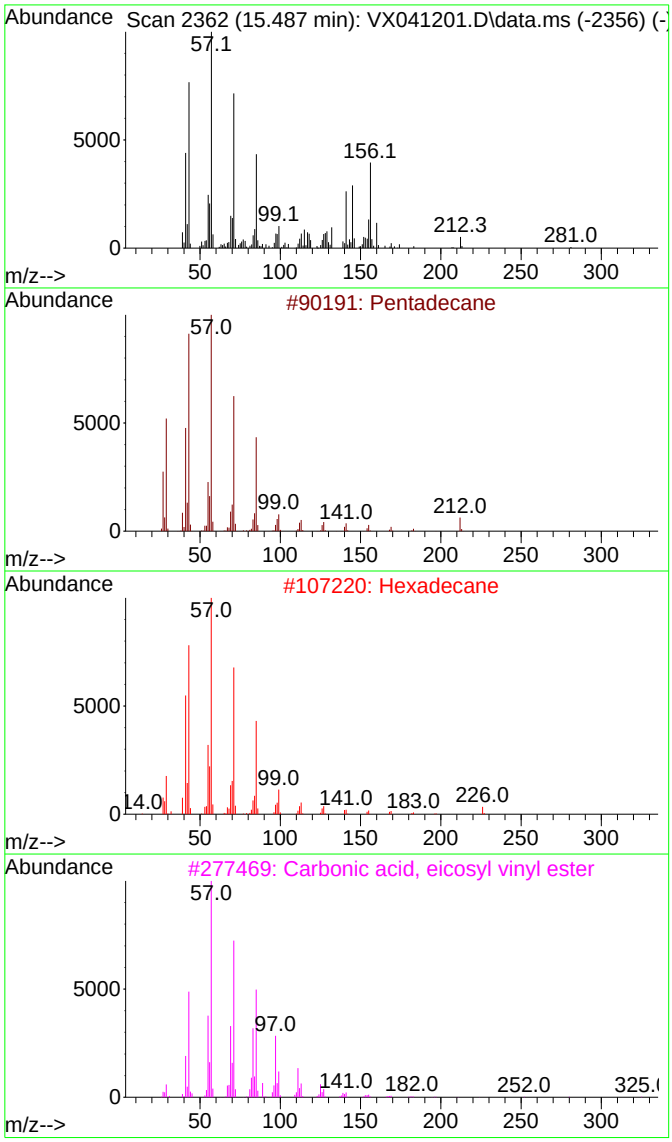
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

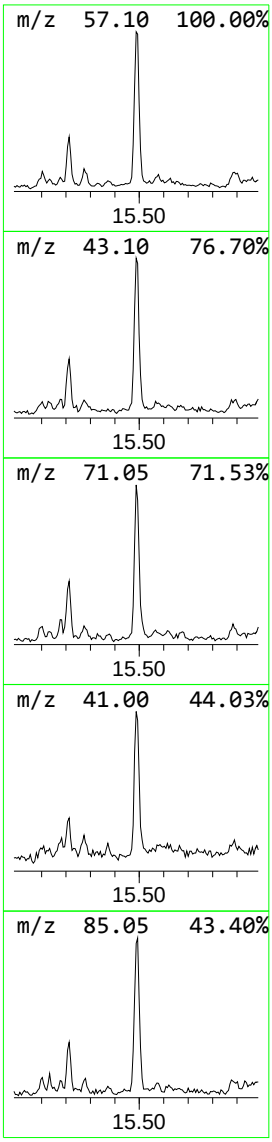
****

Peak Number 5 Pentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.487	6.76 ug/l	113725	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	94
2	Hexadecane	226	C16H34	000544-76-3	42
3	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	41
4	Tetracosane	338	C24H50	000646-31-1	38
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	38





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042224W.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
Sulfur dioxide	1.240	7.2	ug/l	82981	1	5.550	576896	50.0
1-Propene, 2-me...	1.355	8.4	ug/l	97218	1	5.550	576896	50.0
2-Propanethiol,...	3.690	5.7	ug/l	65368	1	5.550	576896	50.0
Cyclohexanol, 5...	13.591	16.3	ug/l	274156	4	12.024	840753	50.0
Pentadecane	15.487	6.8	ug/l	113725	4	12.024	840753	50.0