LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX022323\
Data File : VX034243.D
Acq On : 23 Feb 2023 12:39
Operator : JC/MD
Sample : 01655-09
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31962

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\82X021723W.M
Title : SW846 8260

Signal : TIC: VX034243.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.148	6	10	20	rBV2	149827	176246	1.31%	0.552%
2	2.050	153	158	168	rBV	155126	258779	1.93%	0.811%
3	2.379	206	212	216	rBV	95767	156973	1.17%	0.492%
4	2.965	298	308	323	rBV	1301830	2619831	19.53%	8.207%
5	3.696	415	428	452	rBV	5019689	13416151	100.00%	42.027%
6	4.196	498	510	531	rBV3	246259	772502	5.76%	2.420%
7	4.556	559	569	586	rBV	91424	259162	1.93%	0.812%
8	5.385	695	705	716	rBV2	165576	487040	3.63%	1.526%
9	5.550	723	732	746	rVB2	273893	790478	5.89%	2.476%
10	5.958	787	799	805	rBV	182555	487732	3.64%	1.528%
11	6.043	805	813	838	rVB2	565856	2005398	14.95%	6.282%
12	6.763	921	931	948	rBV	438938	1063458	7.93%	3.331%
13	8.647	1234	1240	1246	rBV	937641	1463706	10.91%	4.585%
14	8.720	1246	1252	1258	rVB	1053651	1659780	12.37%	5.199%
15	10.055	1461	1471	1483	rBV	898932	1234298	9.20%	3.867%
16	10.195	1489	1494	1502	rVB	140262	184070	1.37%	0.577%
17	10.299	1505	1511	1518	rBV	527963	711736	5.31%	2.230%
18	10.640	1560	1567	1581	rBV2	243087	428087	3.19%	1.341%
19	11.079	1634	1639	1645	rBV	726452	925880	6.90%	2.900%
20	12.024	1788	1794	1797	rBV	838226	1141421	8.51%	3.576%
21	12.055	1797	1799	1802	rVV	155967	178692	1.33%	0.560%
22	12.219	1821	1826	1838	rBV	257961	395812	2.95%	1.240%
23	12.408	1852	1857	1863	rBV	258991	347997	2.59%	1.090%
24	12.487	1865	1870	1875	rVB	134298	157683	1.18%	0.494%
25	12.847	1924	1929	1932	rBV	158724	186560	1.39%	0.584%
26	13.774	2075	2081	2088	rVB	187659	249436	1.86%	0.781%
27	14.633	2213	2222	2231	rBV2	98960	163856	1.22%	0.513%

Sum of corrected areas: 31922764

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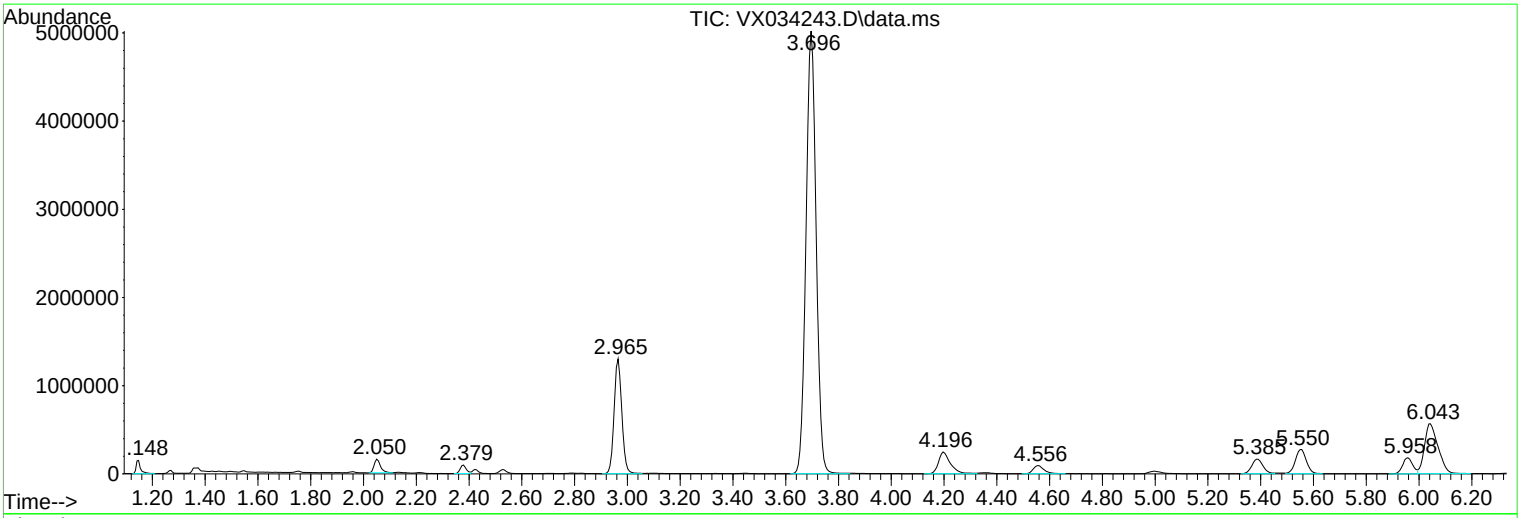
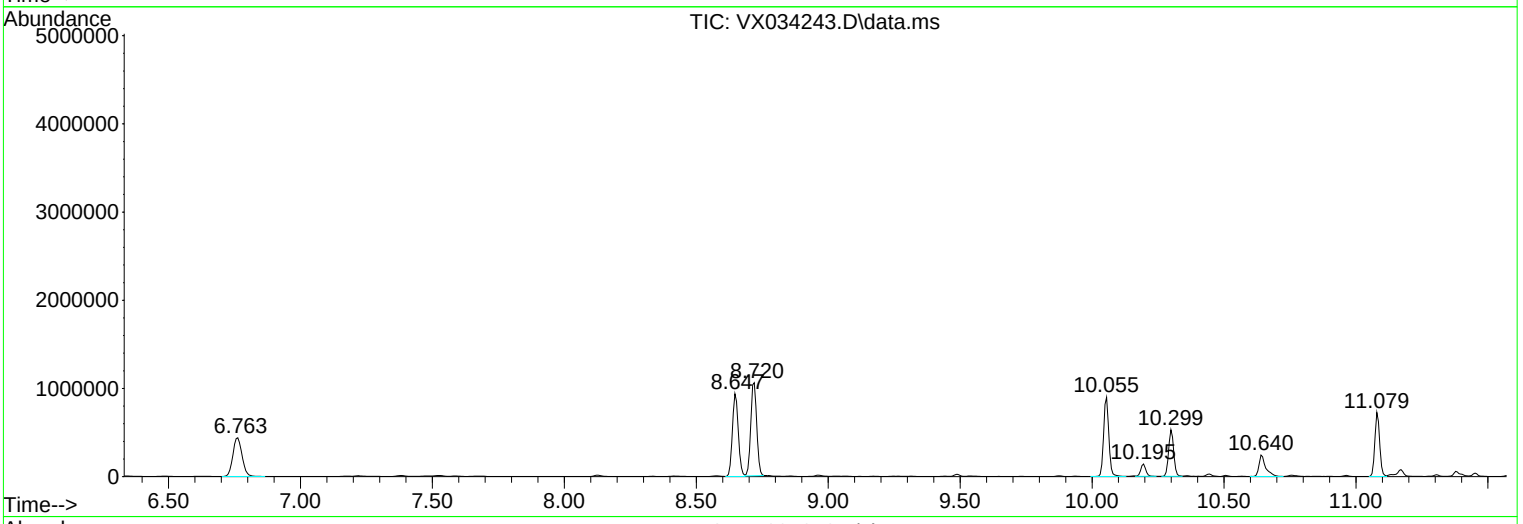
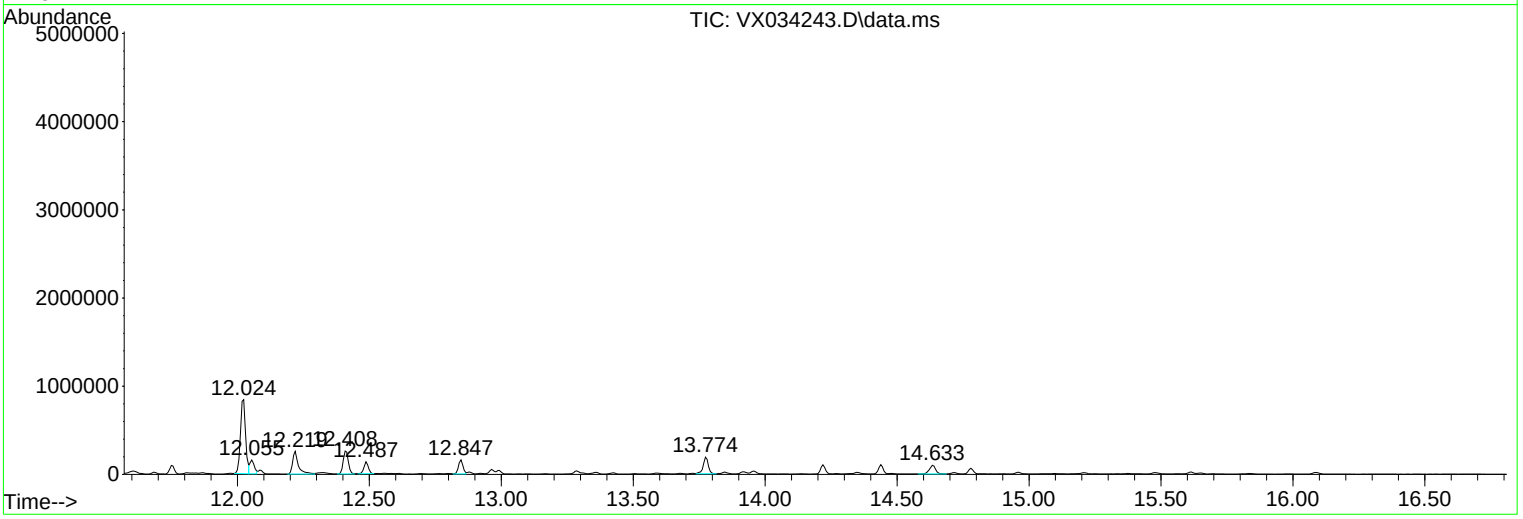
ClientSampleId :
31962

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

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







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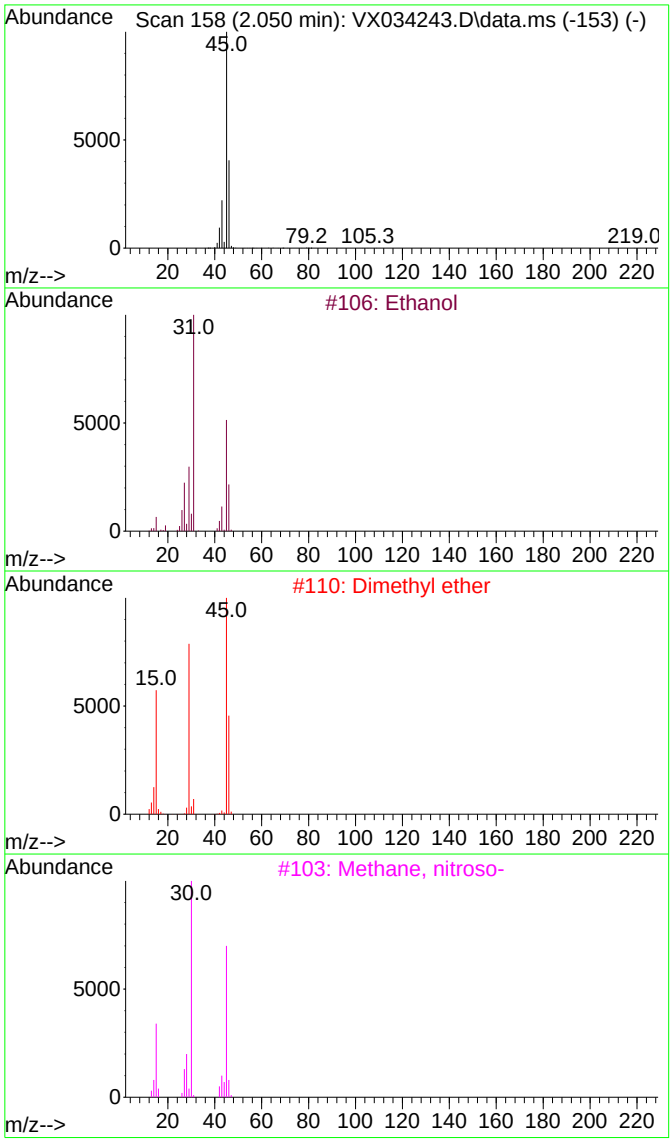
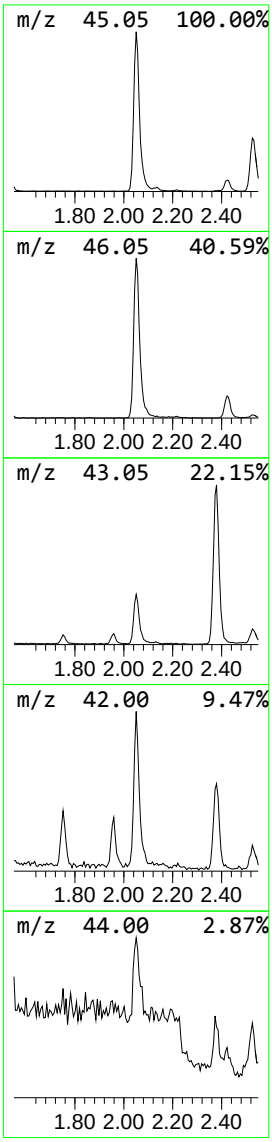
****
Peak Number 2 Ethanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.050	16.37 ug/l	258779	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	64
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	Propanedioic acid, dihydroxy-	136	C3H4O6	000560-27-0	4





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Instrument :
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ClientSampleId :
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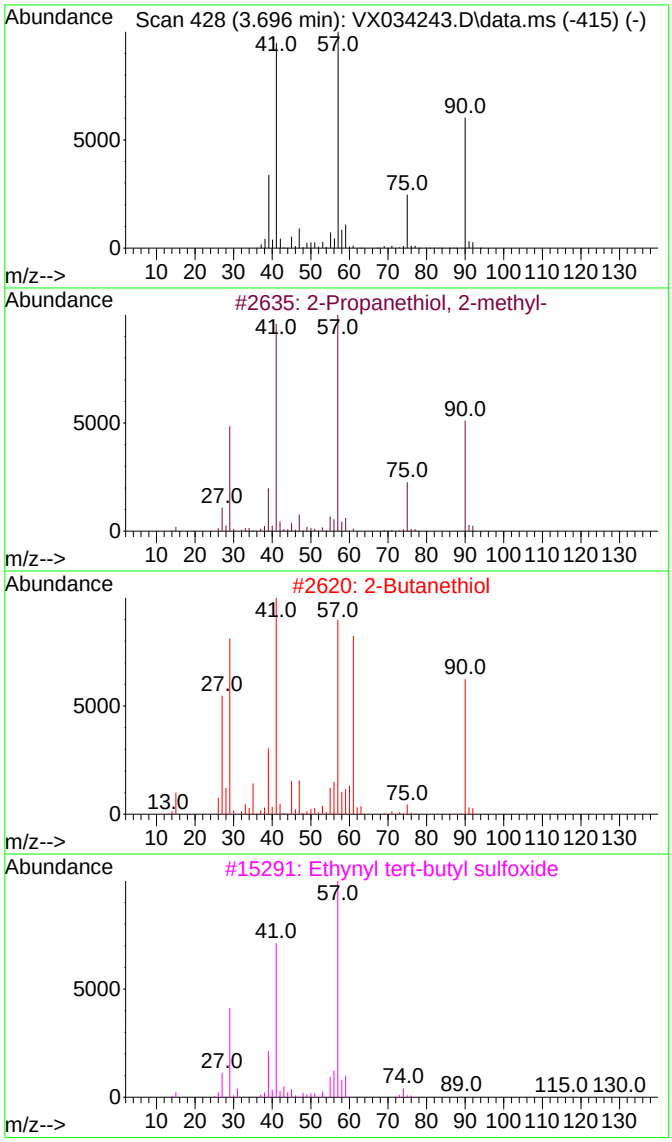
Quant Title : SW846 8260

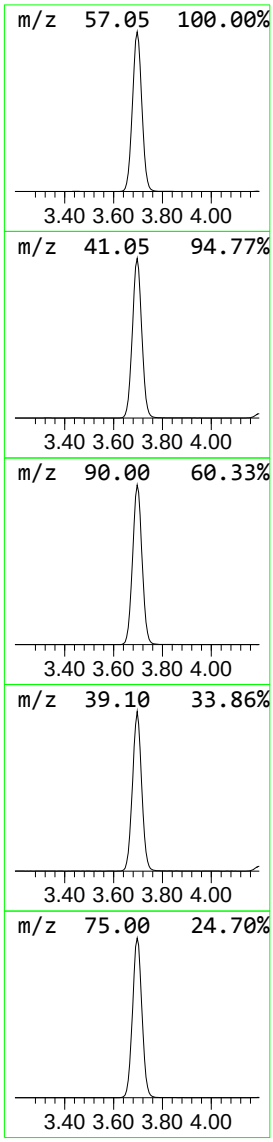
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanethiol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.696	848.61 ug/l	13416200	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	91
2	2-Butanethiol	90	C4H10S	000513-53-1	42
3	Ethynyl tert-butyl sulfoxide	130	C6H10OS	041463-34-7	16
4	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	14
5	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	14





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Instrument :
MSVOA_X
ClientSampleId :
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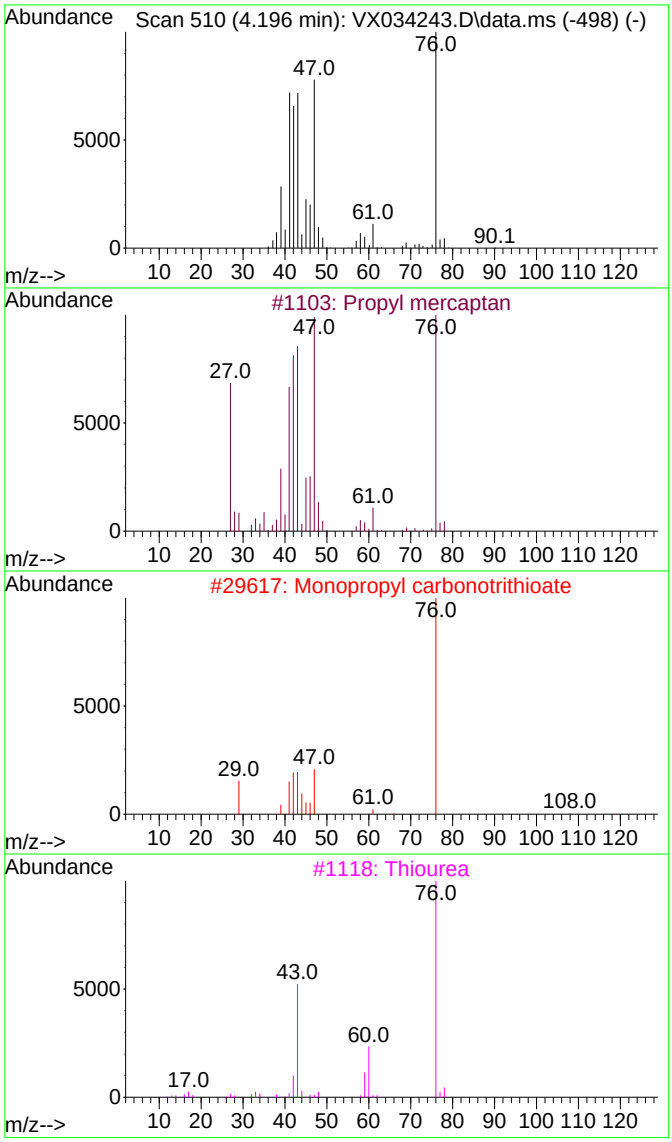
Quant Title : SW846 8260

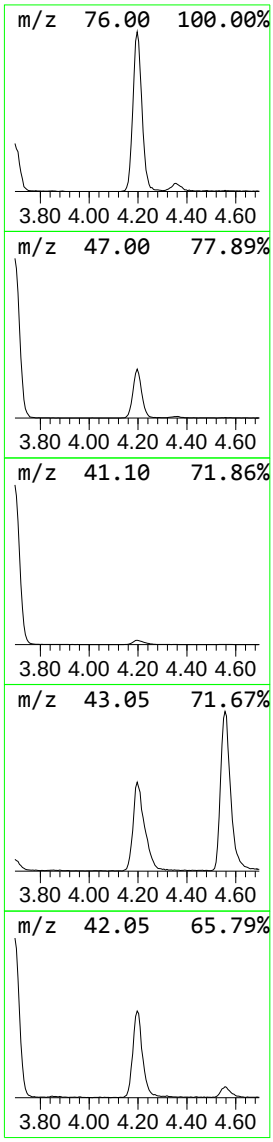
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propyl mercaptan Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.196	48.86 ug/l	772502	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propyl mercaptan	76	C3H8S	000107-03-9	97
2	Monopropyl carbonotrithioate	152	C4H8S3	068060-07-1	74
3	Thiourea	76	CH4N2S	000062-56-6	40
4	Ethane, fluoro-	48	C2H5F	000353-36-6	9
5	Monomethyl carbonotrithioate	124	C2H4S3	001113-26-4	9





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Instrument :
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ClientSampleId :
31962

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

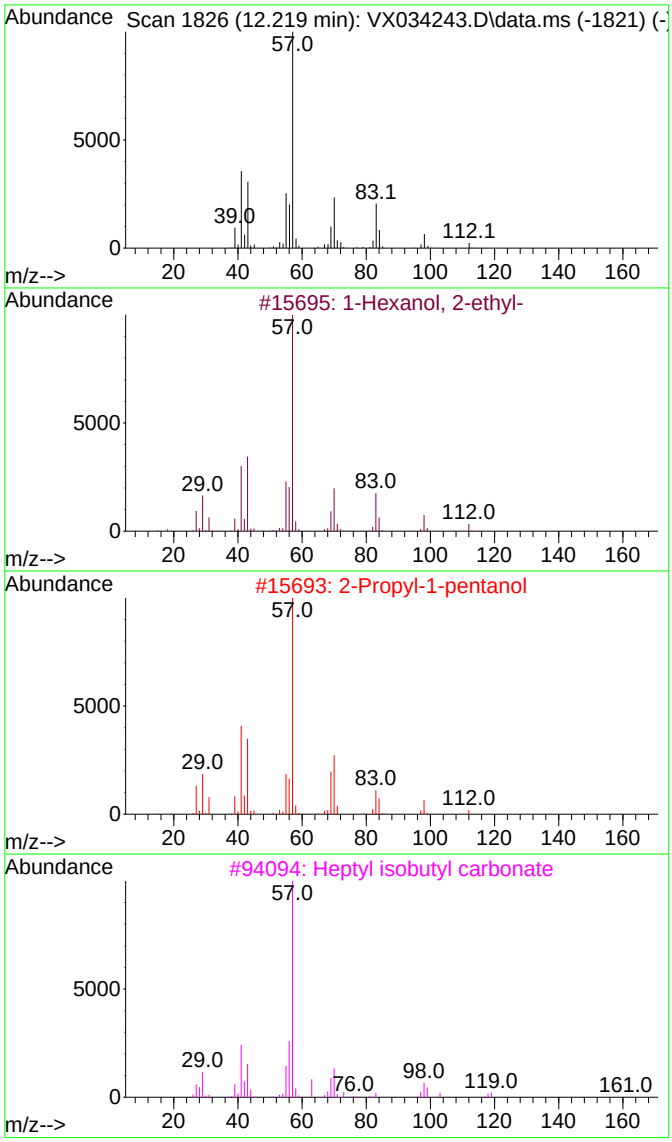
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

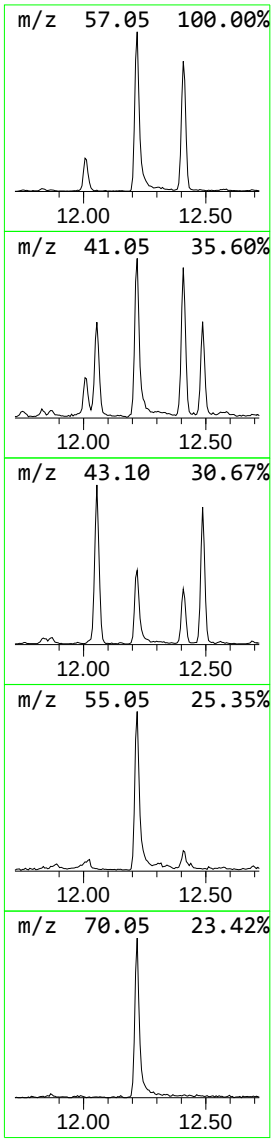
****

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	17.34 ug/l	395812	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	83
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
3	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	50
4	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
5	Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	45





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Instrument :
MSVOA_X
ClientSampleId :
31962

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

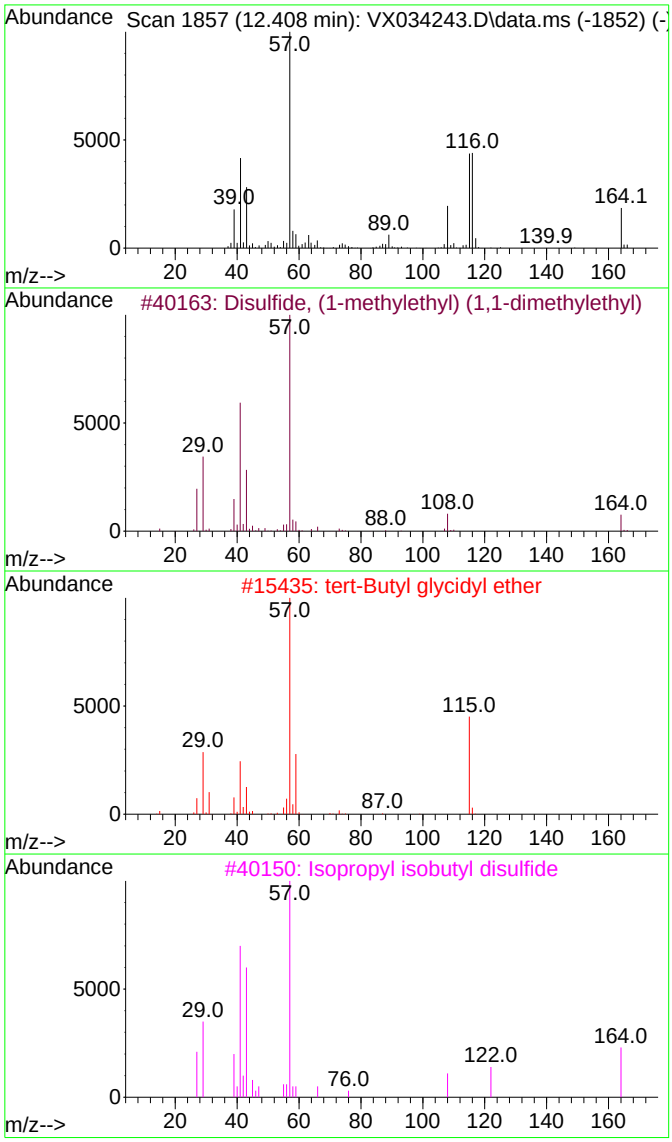
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

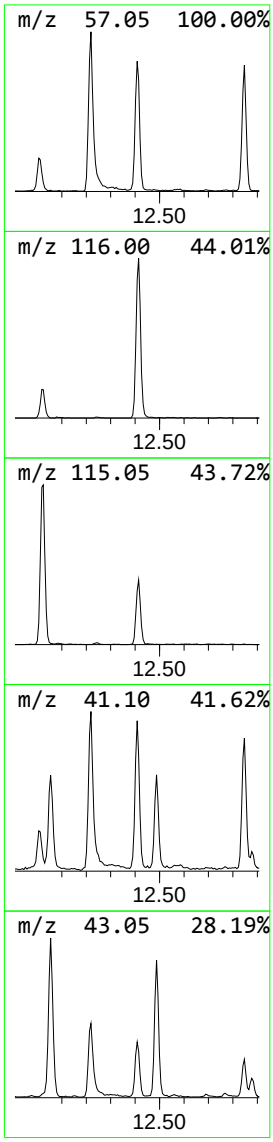
****

Peak Number 6 unknown12.408 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.408	15.24 ug/l	347997	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, (1-methylethyl) (1,1-...	164	C7H16S2	043022-60-2	20
2	tert-Butyl glycidyl ether	130	C7H14O2	007665-72-7	16
3	Isopropyl isobutyl disulfide	164	C7H16S2	067421-82-3	9
4	Disulfide, butyl (1-methylethyl)	164	C7H16S2	072437-53-7	9
5	2-Butanamine, N-methyl-N-nitroso-	116	C5H12N2O	035606-37-2	9





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MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.M
Quant Title : SW846 8260

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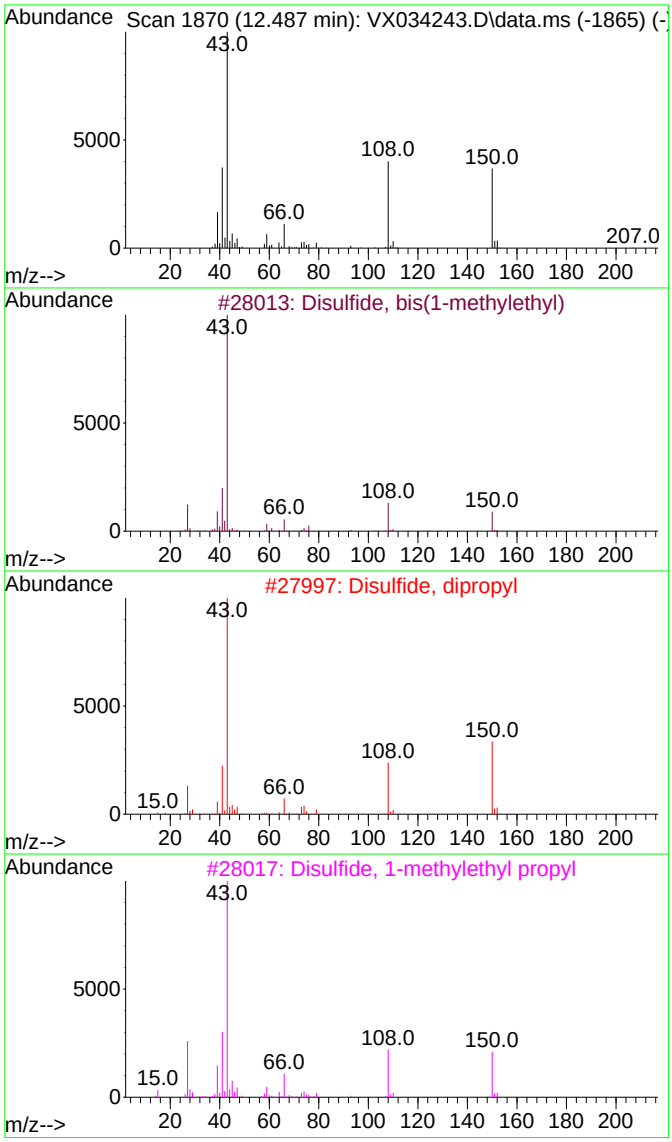
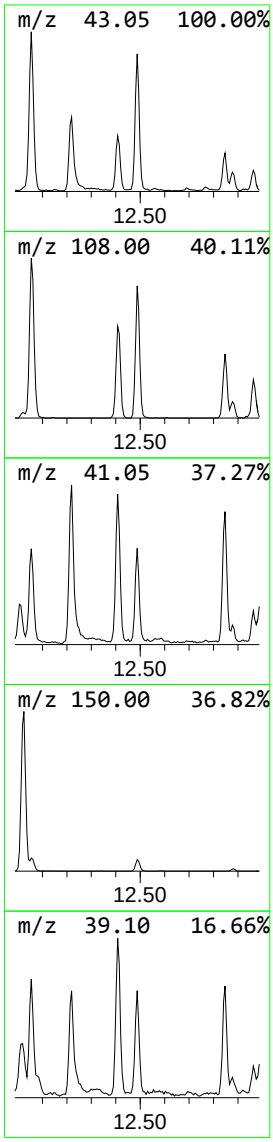
****
Peak Number 7 Disulfide, bis(1-methylethyl) Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.487	6.91 ug/l	157683	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, bis(1-methylethyl)	150	C6H14S2	004253-89-8	72
2	Disulfide, dipropyl	150	C6H14S2	000629-19-6	64
3	Disulfide, 1-methylethyl propyl	150	C6H14S2	033672-51-4	64
4	Disulfide, isopentyl methyl	150	C6H14S2	072437-56-0	35
5	2-Acetoxy-1,1,1-trichloro-4-(4-n...	353	C12H10Cl3NO5	292826-59-6	10





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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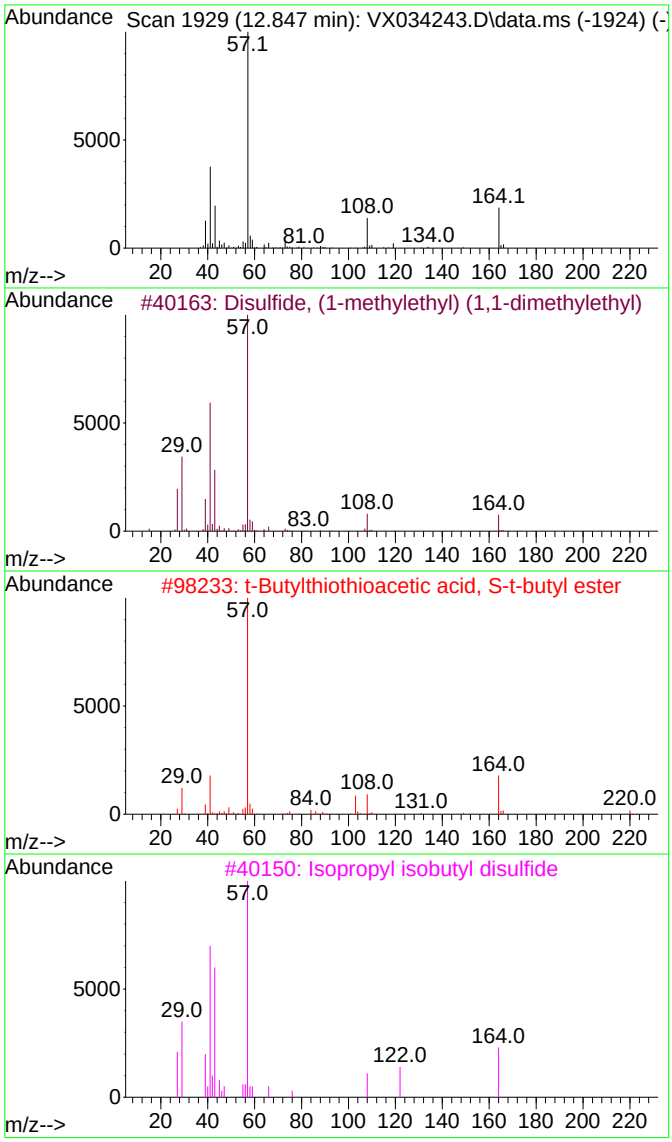
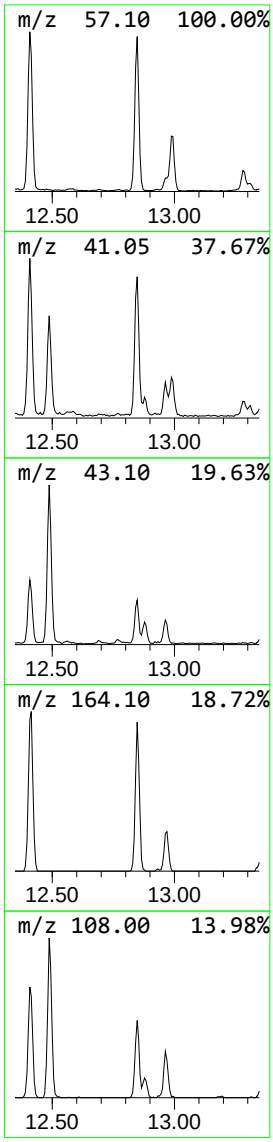
****
Peak Number 8 Disulfide, (1-methylethyl) ... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.847	8.17 ug/l	186560	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, (1-methylethyl) (1,1-...	164	C7H16S2	043022-60-2	64
2	t-Butylthiothioacetic acid, S-t-...	220	C10H20OS2	1000189-14-7	56
3	Isopropyl isobutyl disulfide	164	C7H16S2	067421-82-3	25
4	Propanoic acid, 1,1-dimethylethy...	130	C7H14O2	020487-40-5	17
5	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	12





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TIC Library : C:\Database\NIST20.L
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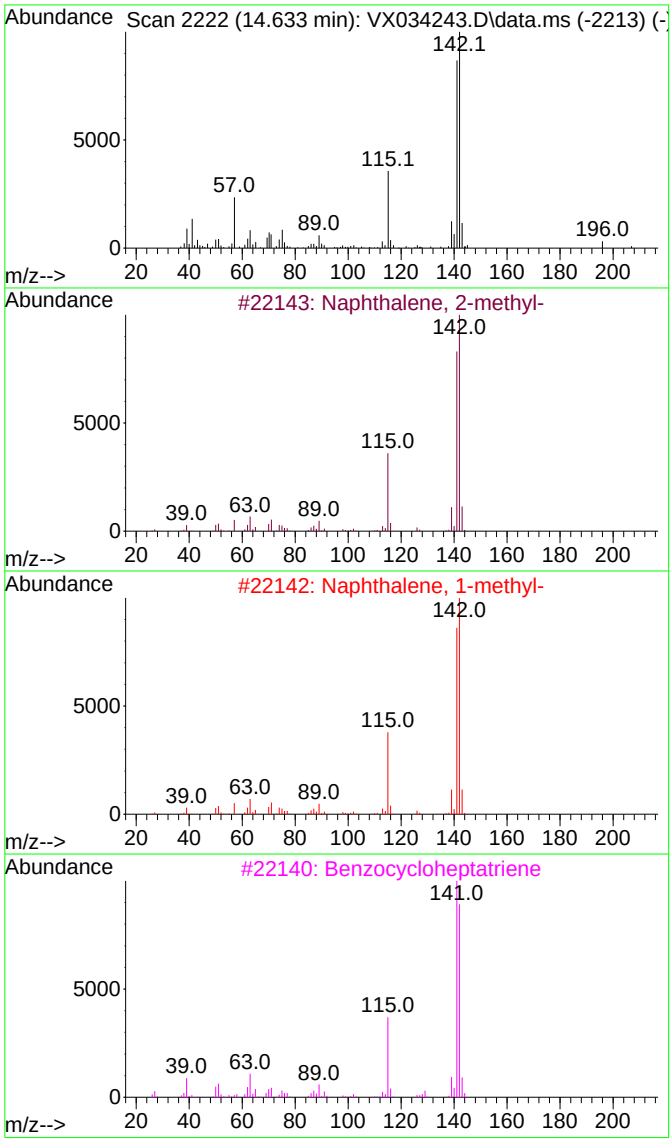
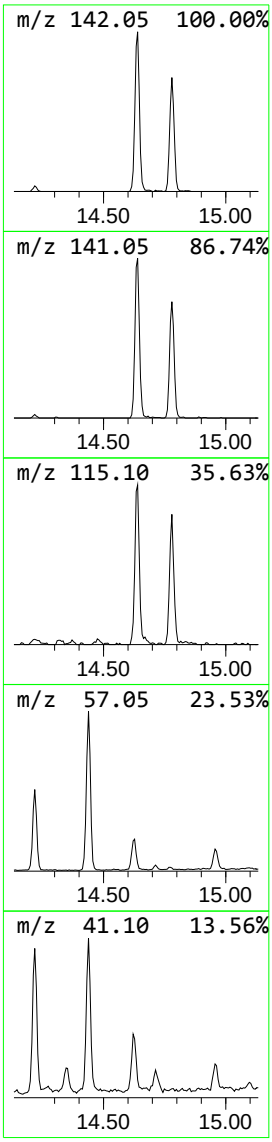
****
Peak Number 9 Naphthalene, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.633	7.18 ug/l	163856	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	97
3	Benzocycloheptatriene	142	C11H10	000264-09-5	95
4	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
5	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91





Tentatively Identified Compound (LSC) summary

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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021723W.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
Ethanol	2.050	16.4	ug/l	258779	1	5.556	790478	50.0
2-Propanethiol,...	3.696	848.6	ug/l	13416200	1	5.556	790478	50.0
Propyl mercaptan	4.196	48.9	ug/l	772502	1	5.556	790478	50.0
1-Hexanol, 2-et...	12.219	17.3	ug/l	395812	4	12.024	1141420	50.0
unknown12.408	12.408	15.2	ug/l	347997	4	12.024	1141420	50.0
Disulfide, bis(...	12.487	6.9	ug/l	157683	4	12.024	1141420	50.0
Disulfide, (1-m...	12.847	8.2	ug/l	186560	4	12.024	1141420	50.0
Naphthalene, 2-...	14.633	7.2	ug/l	163856	4	12.024	1141420	50.0