LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120622\
Data File : VN075586.D
Acq On : 06 Dec 2022 15:50
Operator : JC\MD
Sample : IBLK
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
IBLK

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_N\methods\82N112122W.M
Title : SW846 8260

Signal : TIC: VN075586.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.289	35	40	56	rBV2	36856	132497	2.48%	1.036%
2	2.495	69	75	89	rBV2	69833	197940	3.71%	1.548%
3	4.442	398	406	419	rBV	27485	81461	1.53%	0.637%
4	5.600	575	603	623	rBV2	115485	427347	8.01%	3.342%
5	6.688	772	788	810	rBV	1564986	5336783	100.00%	41.734%
6	7.235	870	881	892	rBV3	33795	99527	1.86%	0.778%
7	7.494	908	925	936	rBV	143752	398923	7.47%	3.120%
8	7.847	973	985	1001	rBV3	36491	99115	1.86%	0.775%
9	8.171	1031	1040	1044	rBV2	95255	213531	4.00%	1.670%
10	8.230	1044	1050	1066	rVB	207954	469167	8.79%	3.669%
11	8.588	1097	1111	1121	rBV2	77995	244385	4.58%	1.911%
12	9.106	1189	1199	1211	rBV	298980	618108	11.58%	4.834%
13	10.571	1439	1448	1453	rBV	176464	370967	6.95%	2.901%
14	10.635	1453	1459	1473	rVB	280481	568254	10.65%	4.444%
15	11.870	1655	1669	1678	rVB	379864	696868	13.06%	5.450%
16	11.965	1678	1685	1693	rVB	49136	84756	1.59%	0.663%
17	12.070	1695	1703	1711	rBV	181393	340774	6.39%	2.665%
18	12.400	1751	1759	1765	rBV	89603	166190	3.11%	1.300%
19	12.853	1829	1836	1846	rVB	271854	479772	8.99%	3.752%
20	13.117	1863	1881	1897	rBV6	105344	470862	8.82%	3.682%
21	13.341	1900	1919	1932	rBV	153011	338516	6.34%	2.647%
22	13.794	1988	1996	2005	rBV	374435	658047	12.33%	5.146%
23	13.876	2005	2010	2017	rVB	77889	126755	2.38%	0.991%
24	14.023	2027	2035	2053	rVB	19426	101416	1.90%	0.793%
25	14.611	2123	2135	2142	rBV2	31520	65705	1.23%	0.514%

Sum of corrected areas: 12787666

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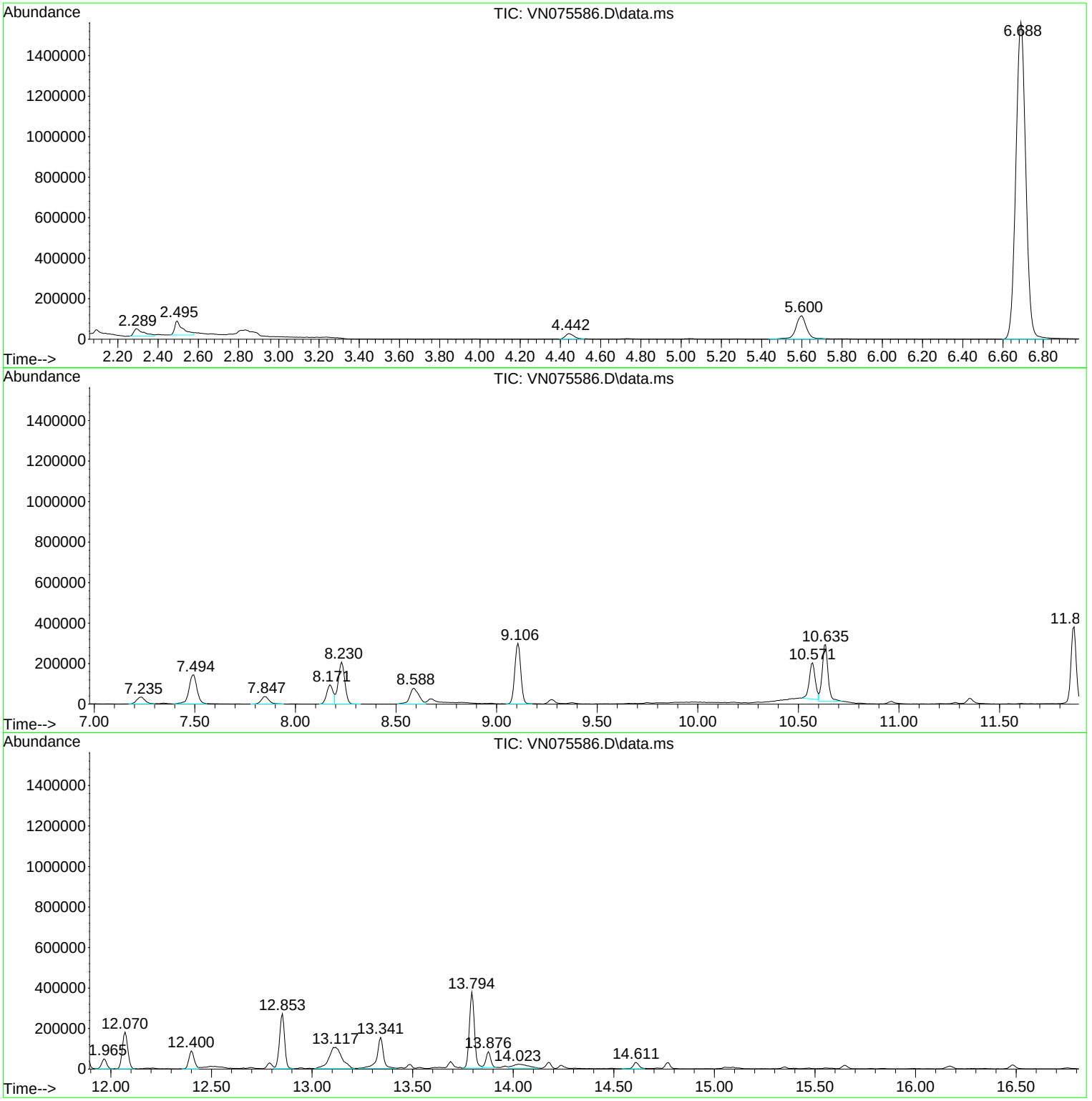
ClientSampleId :
IBLK

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

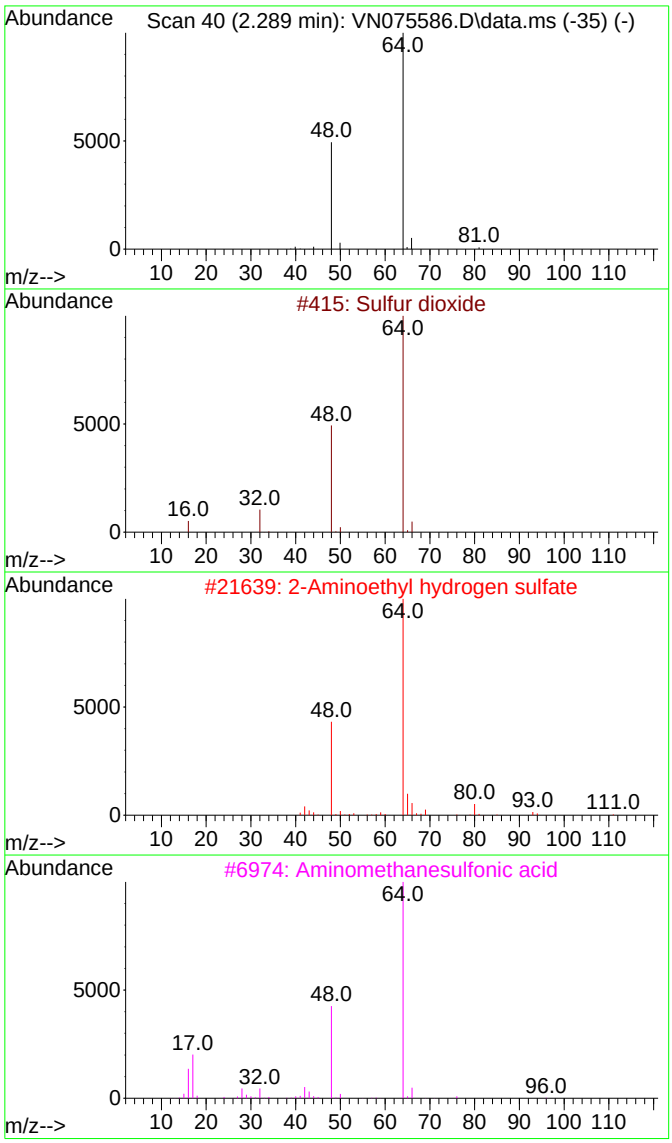
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

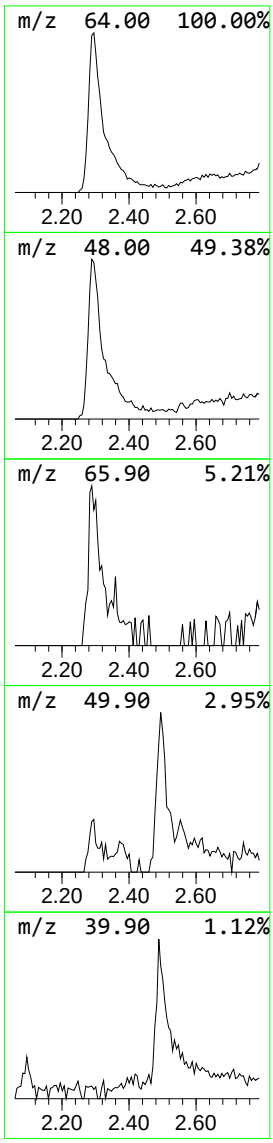
****

Peak Number 1 Sulfur dioxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.289	14.12 ug/l	132497	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4





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ALS Vial : 1 Sample Multiplier: 1

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ClientSampleId :
IBLK

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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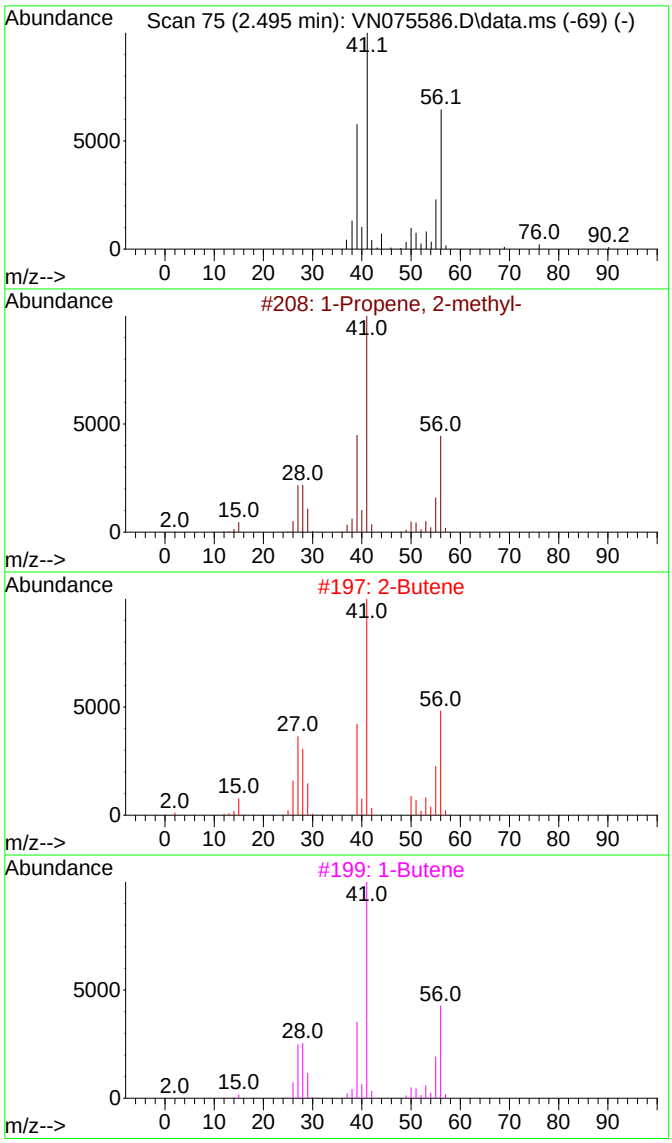
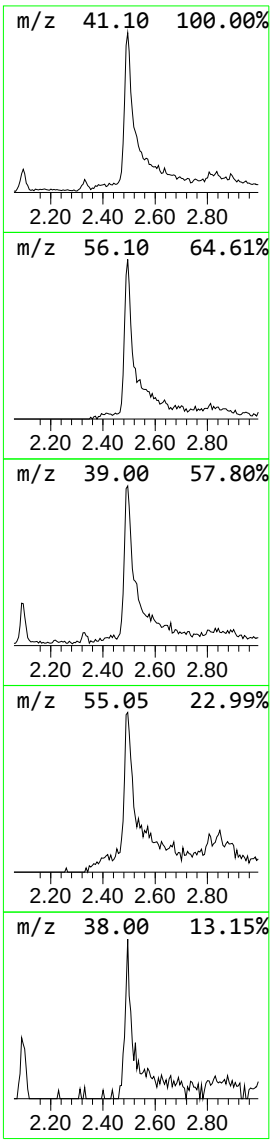
****
Peak Number 2 1-Propene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.495	21.09 ug/l	197940	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-	56	C4H8	000115-11-7	86
2	2-Butene	56	C4H8	000107-01-7	59
3	1-Butene	56	C4H8	000106-98-9	53
4	Allyl chloride	76	C3H5Cl	000107-05-1	47
5	Cyclobutane	56	C4H8	000287-23-0	46





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Instrument :
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ClientSampleId :
IBLK

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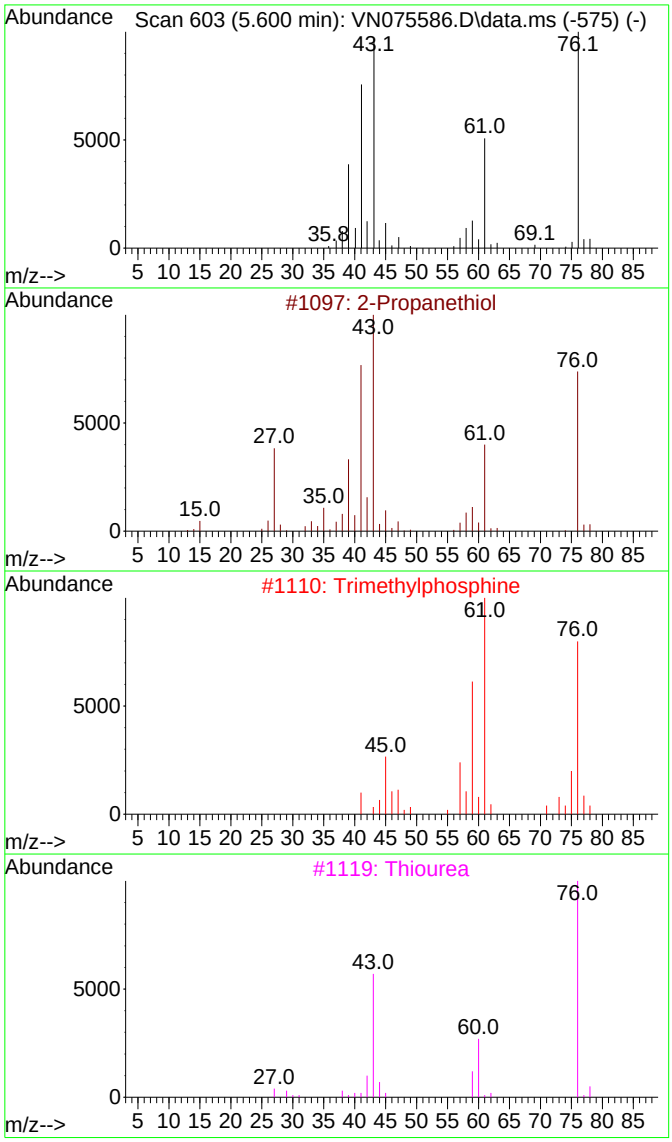
Quant Title : SW846 8260

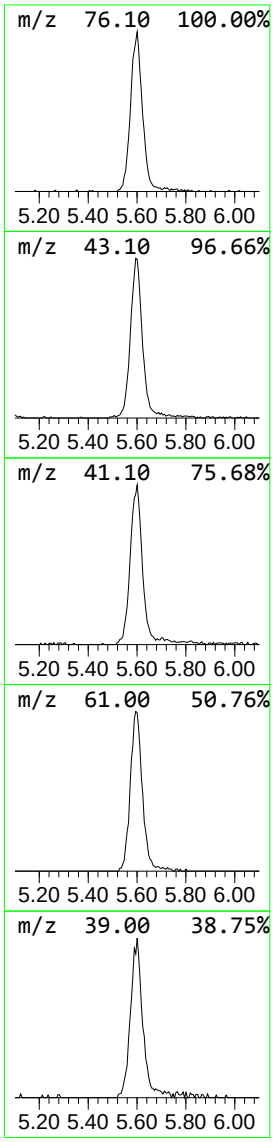
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanethiol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.600	45.54 ug/l	427347	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol	76	C3H8S	000075-33-2	90
2	Trimethylphosphine	76	C3H9P	000594-09-2	78
3	Thiourea	76	CH4N2S	000062-56-6	59
4	Isopropyl phosphine	76	C3H9P	004538-29-8	59
5	Propane, 1,3-dichloro-	112	C3H6Cl2	000142-28-9	36





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ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
IBLK

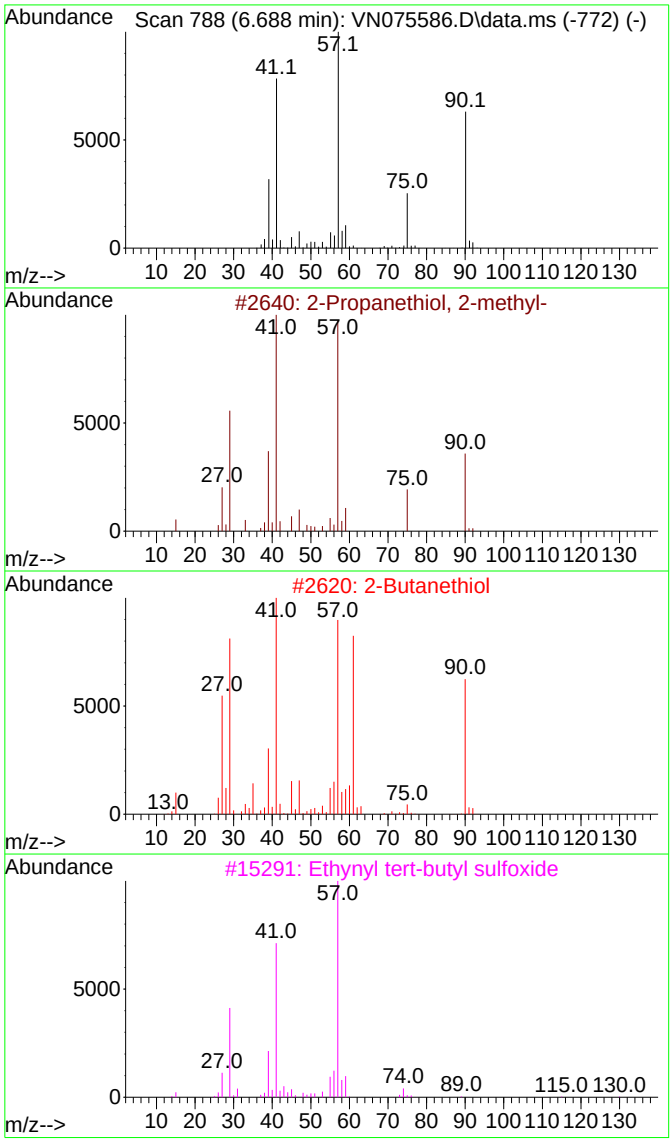
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N112122W.M
Quant Title : SW846 8260

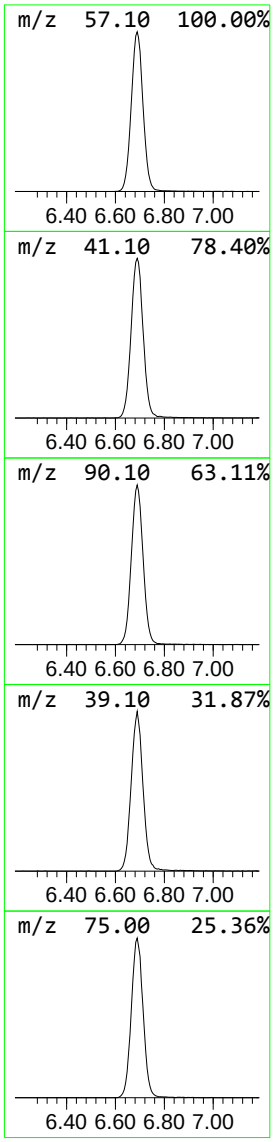
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Propanethiol, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.688	568.75 ug/l	5336780	Pentafluorobenzene	8.230

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-bromo-2-methyl-	136	C4H9Br	000507-19-7	14
5	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	14





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TIC Library : C:\Database\NIST20.L
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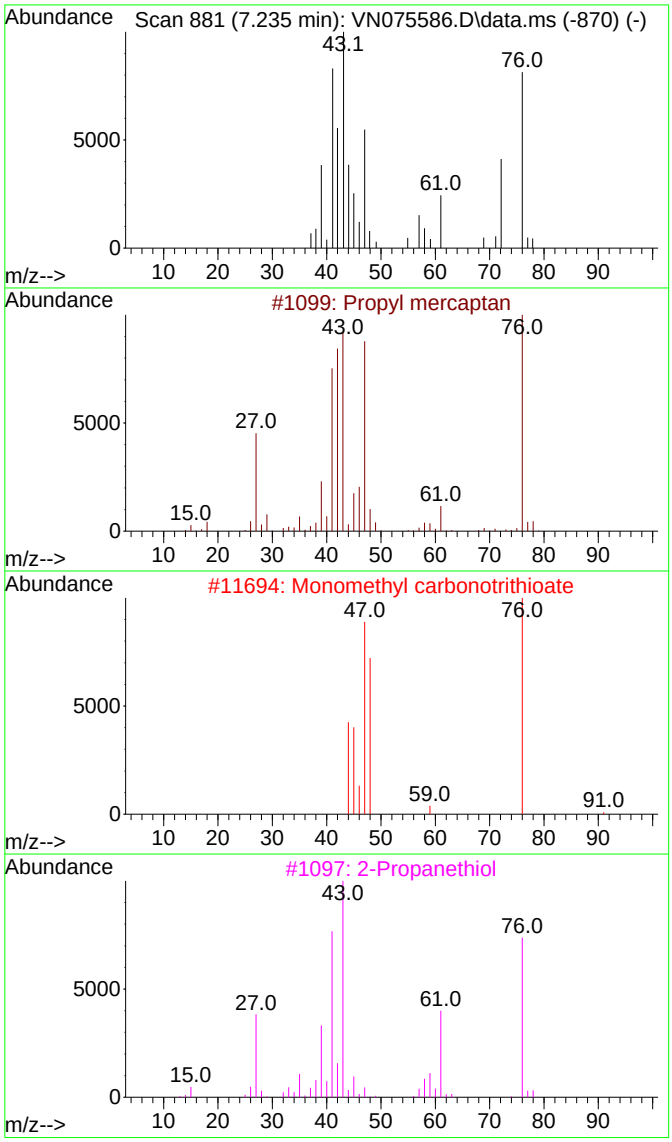
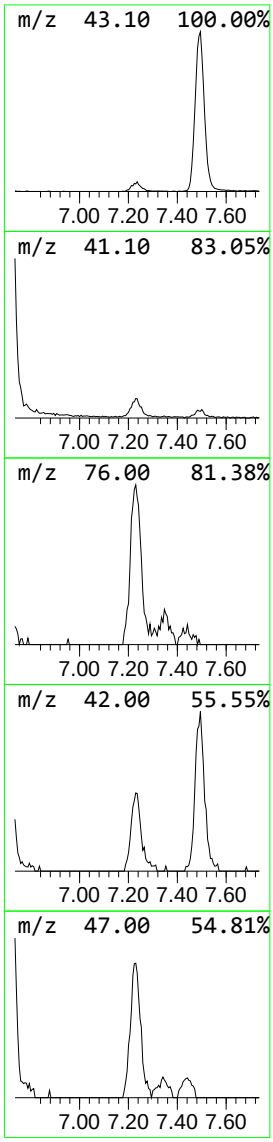
****
Peak Number 5 Propyl mercaptan Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.235	10.61 ug/l	99527	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propyl mercaptan	76	C3H8S	000107-03-9	76
2	Monomethyl carbonotrithioate	124	C2H4S3	001113-26-4	56
3	2-Propanethiol	76	C3H8S	000075-33-2	9
4	Thiourea	76	CH4N2S	000062-56-6	9
5	Isopropyl phosphine	76	C3H9P	004538-29-8	9





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Instrument :
MSVOA_N
ClientSampleId :
IBLK

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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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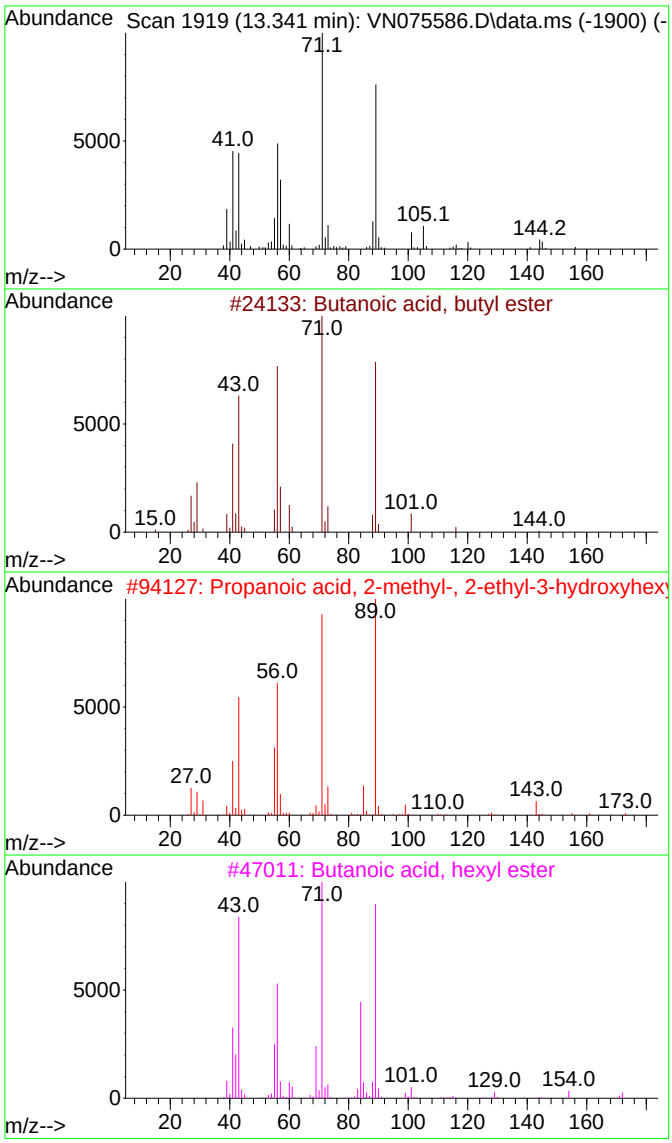
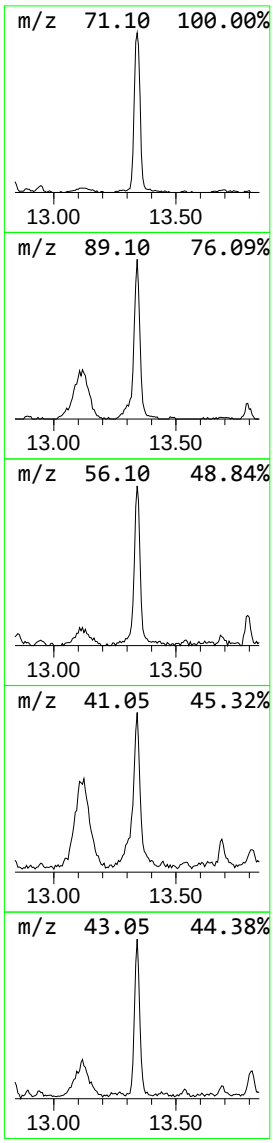
****
Peak Number 7 Butanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	25.72 ug/l	338516	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	83
2	Propanoic acid, 2-methyl-, 2-eth...	216	C12H24O3	074367-31-0	78
3	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	72
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
5	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	72





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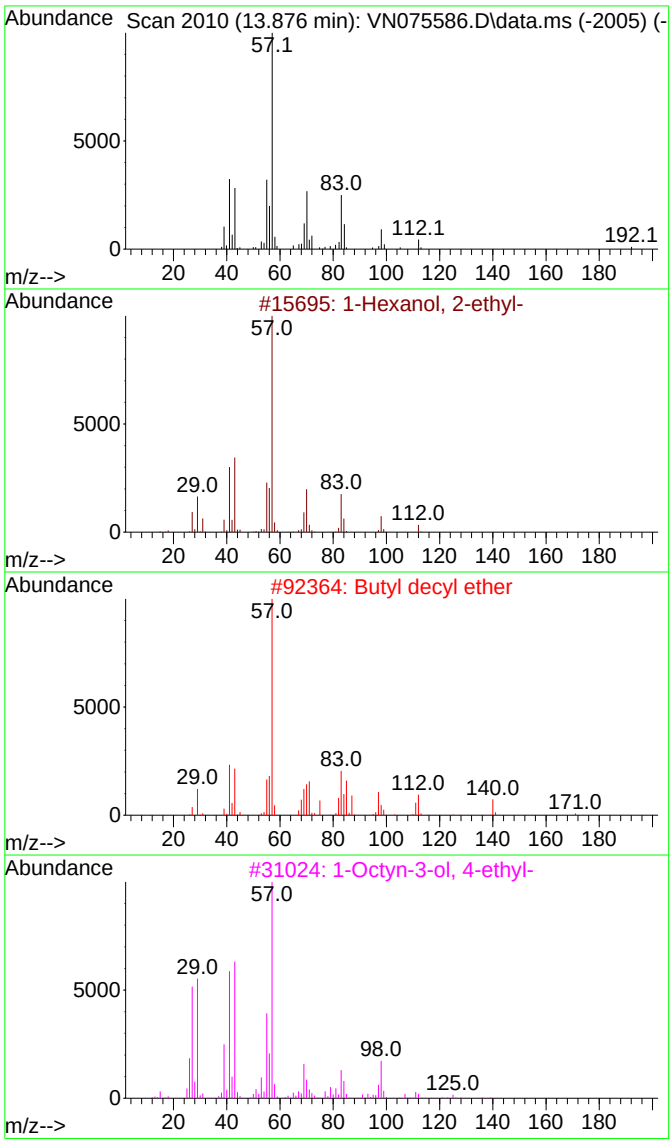
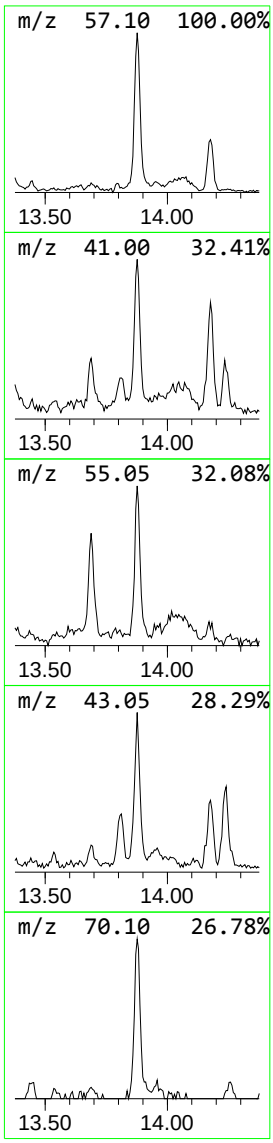
****
Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.876	9.63 ug/l	126755	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2	Butyl decyl ether	214	C14H30O	1000406-40-2	50
3	1-Octyn-3-ol, 4-ethyl-	154	C10H18O	005877-42-9	50
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	47





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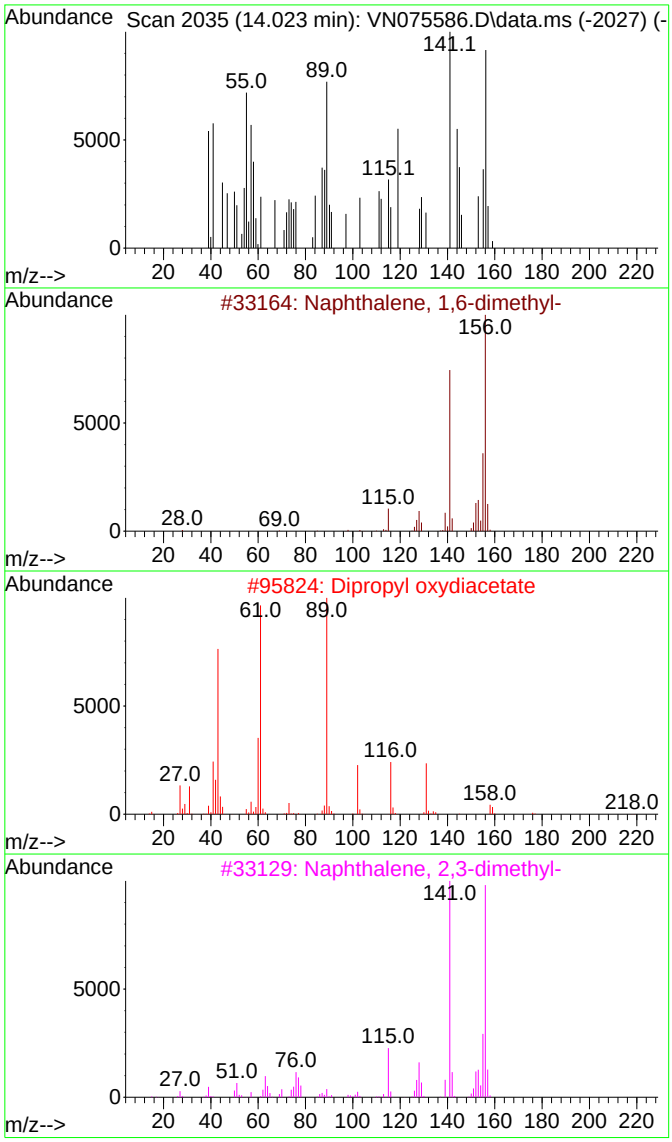
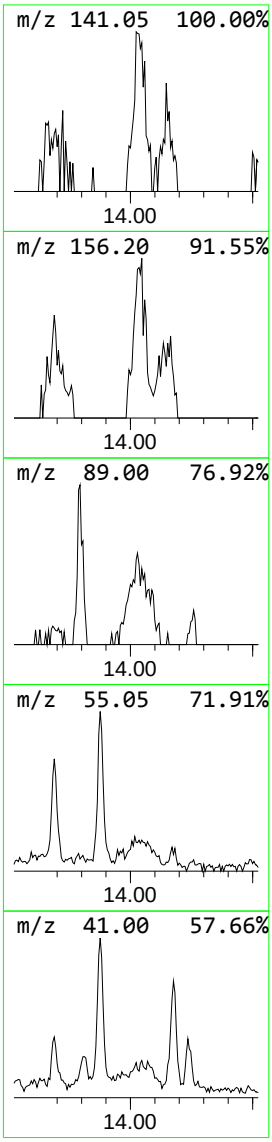
****
Peak Number 9 unknown14.023 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.023	7.71 ug/l	101416	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	47
2	Dipropyl oxydiacetate	218	C10H18O5	085668-79-7	25
3	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	18
4	Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	18
5	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	14





Tentatively Identified Compound (LSC) summary

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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	2.289	14.1	ug/l	132497	1	8.230	469167	50.0
1-Propene, 2-me...	2.495	21.1	ug/l	197940	1	8.230	469167	50.0
2-Propanethiol	5.600	45.5	ug/l	427347	1	8.230	469167	50.0
2-Propanethiol,...	6.688	568.8	ug/l	5336780	1	8.230	469167	50.0
Propyl mercaptan	7.235	10.6	ug/l	99527	1	8.230	469167	50.0
Butanoic acid, ...	13.341	25.7	ug/l	338516	4	13.794	658047	50.0
1-Hexanol, 2-et...	13.876	9.6	ug/l	126755	4	13.794	658047	50.0
unknown14.023	14.023	7.7	ug/l	101416	4	13.794	658047	50.0