LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
Data File : VX020752.D
Acq On : 26 Jan 2021 14:44
Operator : JC/SP
Sample : M1189-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 41089

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\82X012521W.M
Title : SW846 8260

Signal : TIC: VX020752.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.160	9	12	23	rVB	588849	520603	27.33%	3.704%
2	3.007	307	315	331	rBV	59899	133588	7.01%	0.950%
3	3.757	426	438	454	rBV2	297450	842181	44.22%	5.992%
4	4.300	512	527	541	rBV2	206337	595629	31.27%	4.237%
5	5.464	705	718	733	rBV2	220062	625042	32.82%	4.447%
6	5.629	733	745	757	rVV	371458	1034845	54.33%	7.362%
7	6.031	797	811	819	rBV	238275	617391	32.41%	4.392%
8	6.830	931	942	955	rBV	579895	1354720	71.13%	9.638%
9	7.263	1001	1013	1027	rBV	54688	135751	7.13%	0.966%
10	8.695	1240	1248	1254	rBV	1274982	1904681	100.00%	13.551%
11	8.762	1254	1259	1264	rVB	102281	156808	8.23%	1.116%
12	10.091	1471	1477	1488	rBV	1186922	1675514	87.97%	11.920%
13	10.341	1512	1518	1524	rBV	129607	171389	9.00%	1.219%
14	11.122	1640	1646	1651	rBV	991616	1298553	68.18%	9.238%
15	11.719	1739	1744	1751	rBV	164282	200785	10.54%	1.428%
16	11.902	1770	1774	1783	rVB	61524	81656	4.29%	0.581%
17	12.024	1786	1794	1796	rBV	175338	222767	11.70%	1.585%
18	12.061	1796	1800	1808	rVB	1320490	1621155	85.11%	11.533%
19	12.256	1827	1832	1843	rBV	195943	312155	16.39%	2.221%
20	13.444	2014	2027	2040	rBV5	34116	154876	8.13%	1.102%
21	13.646	2052	2060	2069	rBV3	49201	109289	5.74%	0.778%
22	13.816	2084	2088	2094	rVB	91830	117415	6.16%	0.835%
23	13.883	2095	2099	2106	rBV	62518	82356	4.32%	0.586%
24	13.950	2106	2110	2117	rBV	61420	87006	4.57%	0.619%

Sum of corrected areas: 14056155

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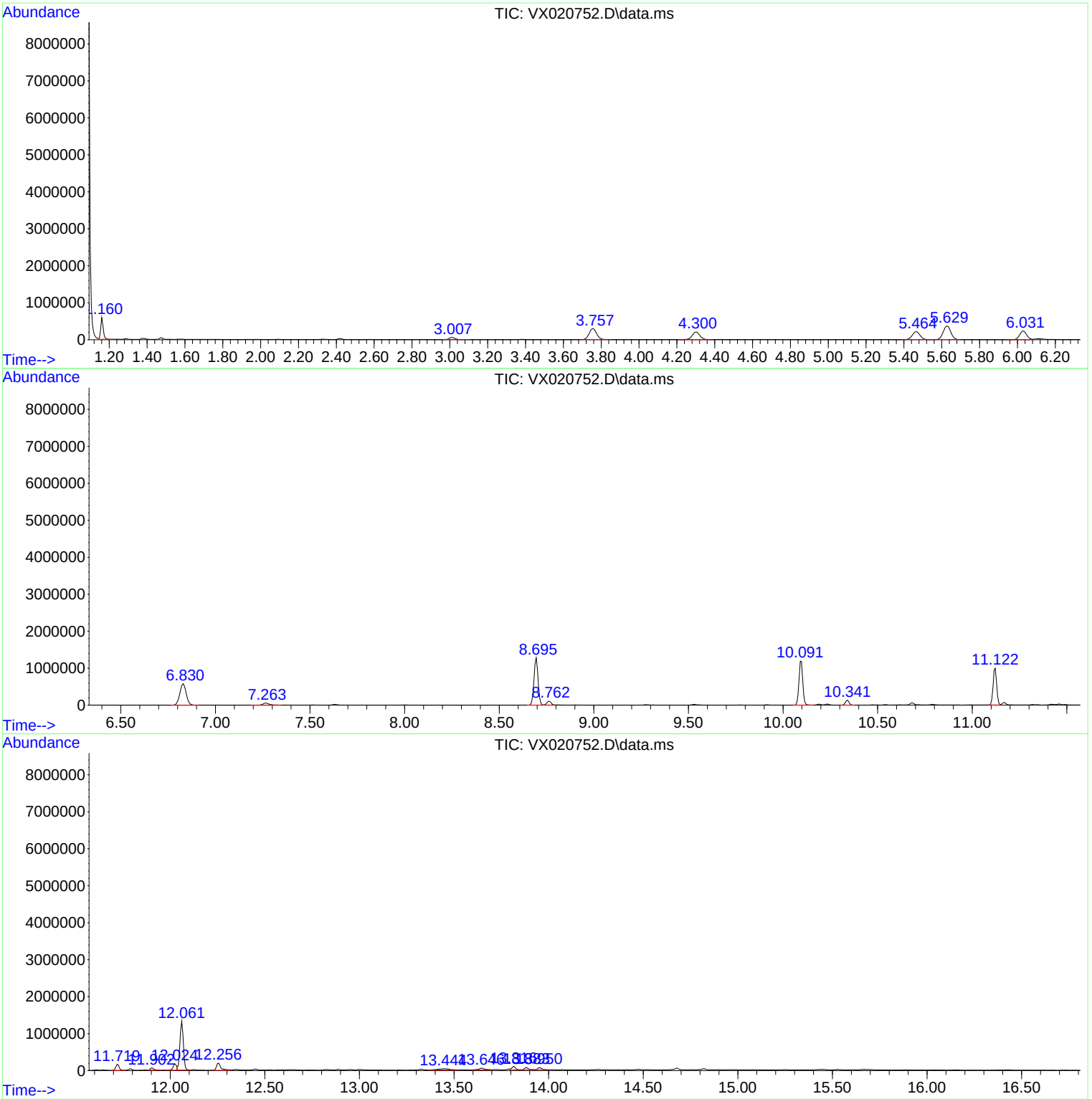
Instrument :
MSVOA_X
ClientSampleId :
41089

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Instrument : MSVOA_X
ClientSampleId : 41089

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

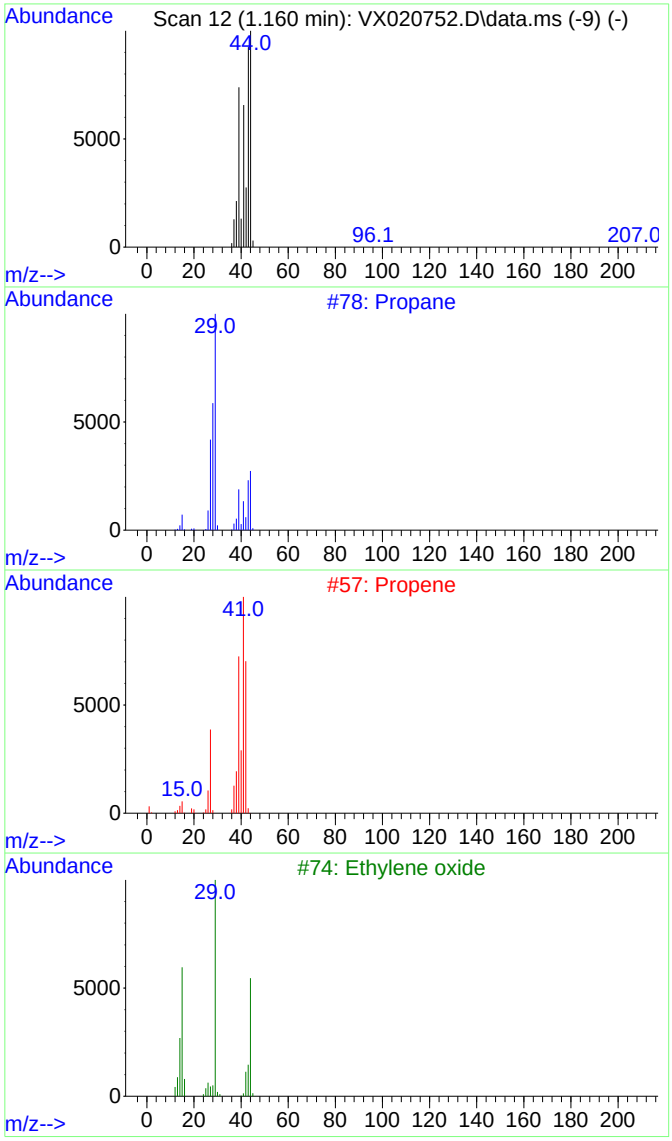
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

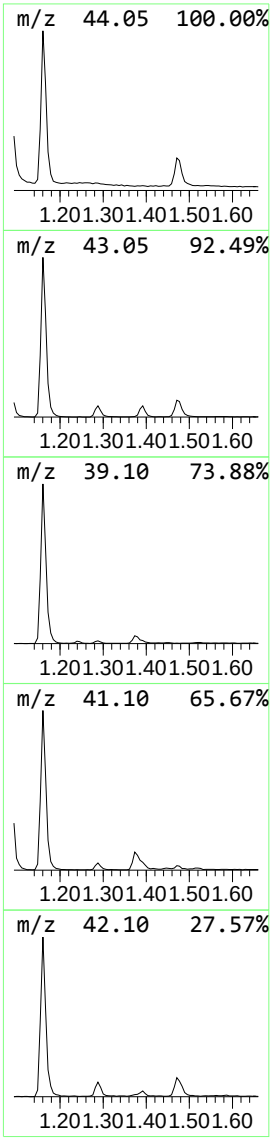
****

Peak Number 1 Propane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.160	25.15 ug/l	520603	Pentafluorobenzene	5.629

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	90
2	Propene	42	C3H6	000115-07-1	9
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Cyclopropene	40	C3H4	002781-85-3	2
5	Alanine	89	C3H7NO2	000056-41-7	2





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Sample : M1189-13
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 41089

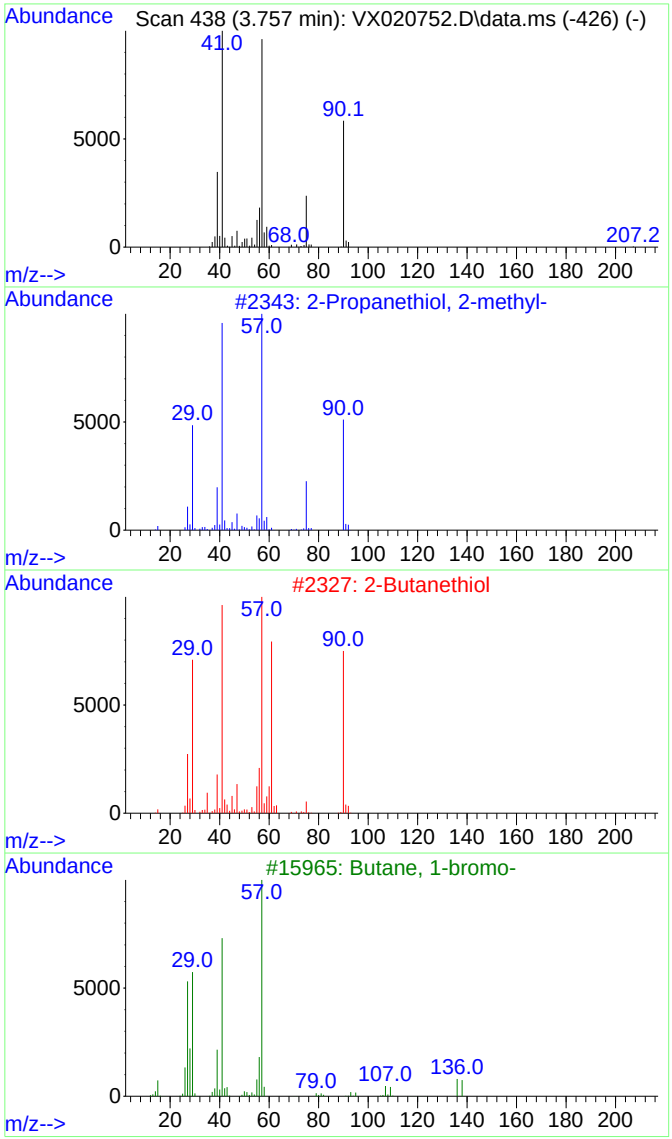
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

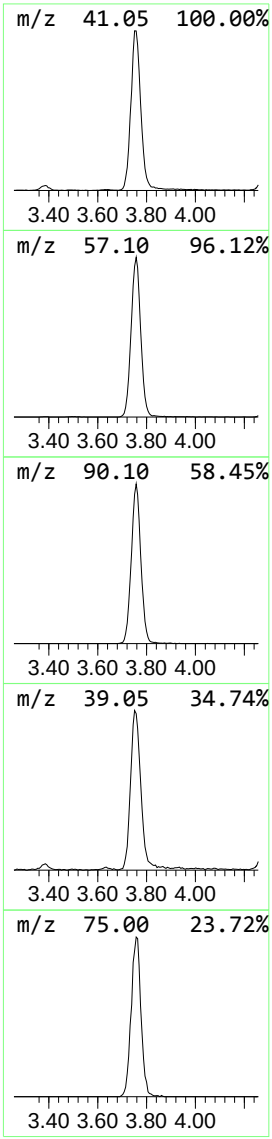
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.757	40.69 ug/l	842181	Pentafluorobenzene	5.629

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	45
3	Butane, 1-bromo-	136	C4H9Br	000109-65-9	22
4	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	22
5	2-Heptanethiol, 2-methyl-	146	C8H18S	000763-20-2	16





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ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 41089

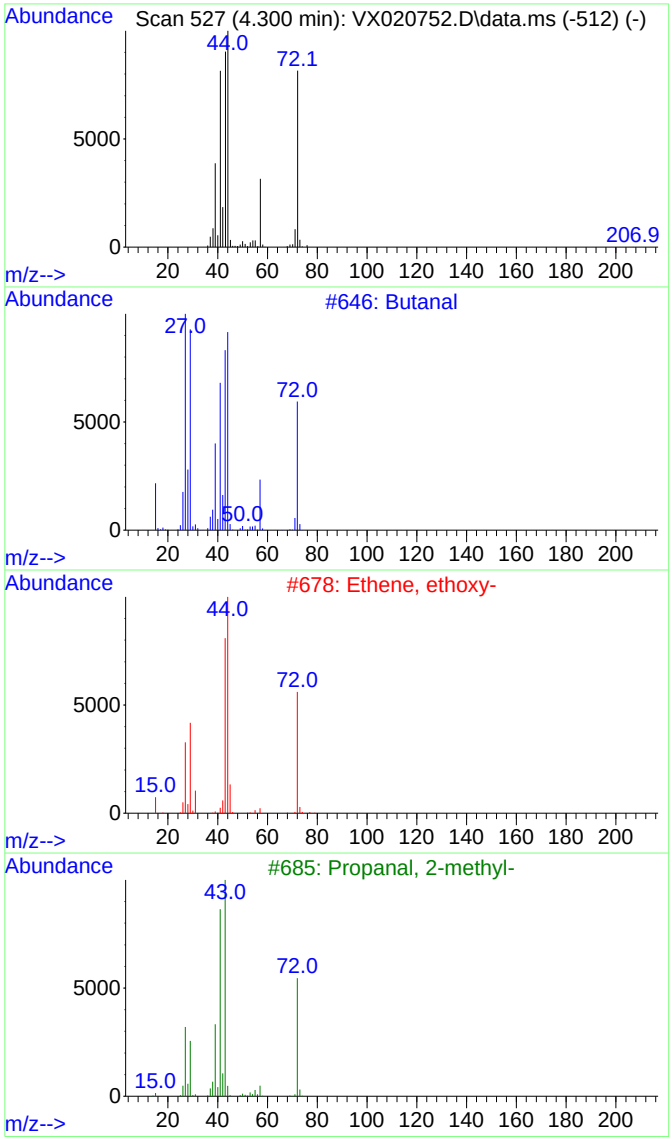
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

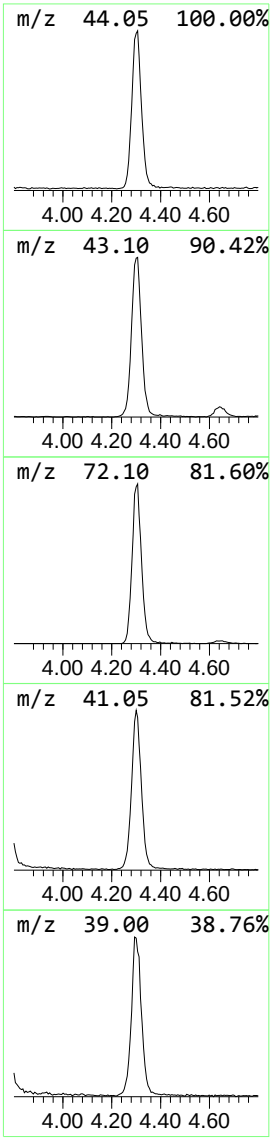
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.300	28.78 ug/l	595629	Pentafluorobenzene	5.629

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	53
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43
5	Isobutylene epoxide	72	C4H8O	000558-30-5	27





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ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 41089

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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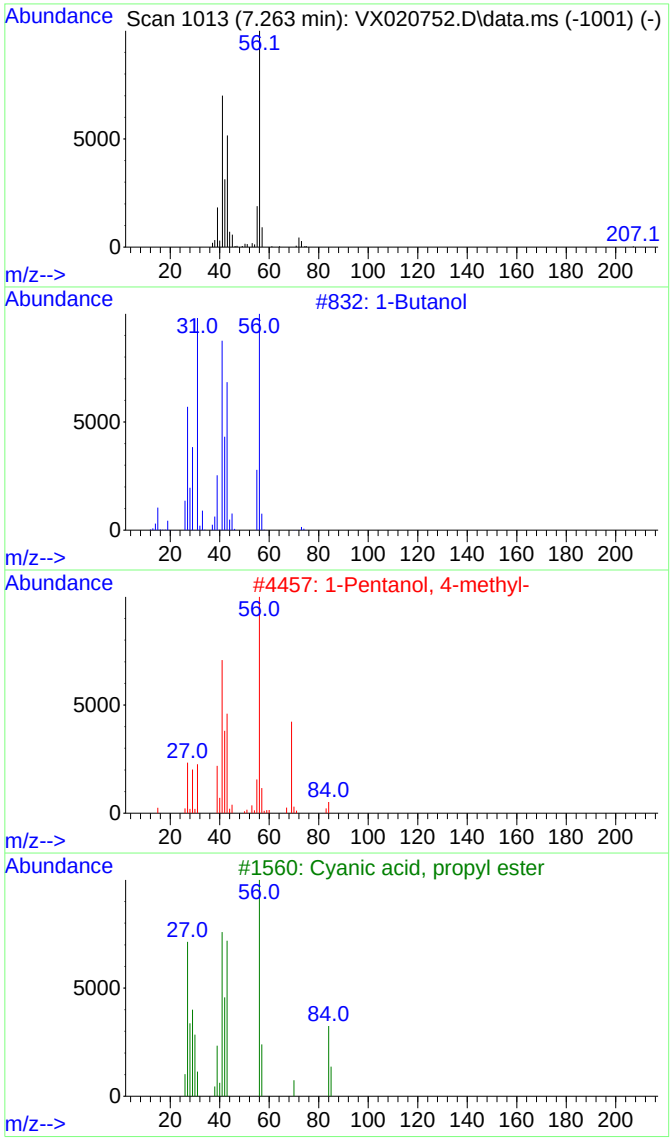
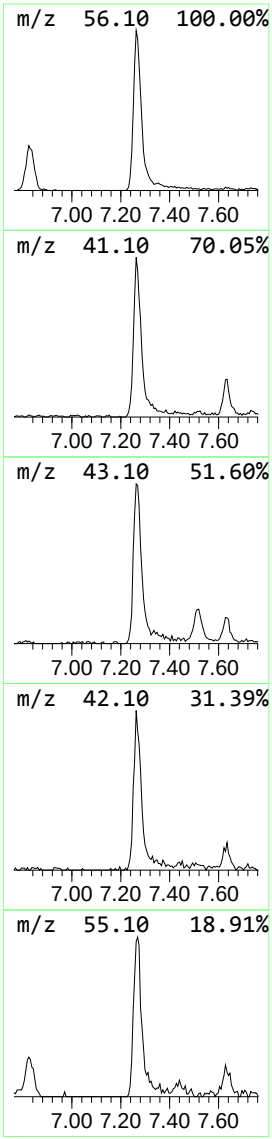
****

Peak Number 4 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.263	5.01 ug/l	135751	1,4-Difluorobenzene	6.830

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	80
2	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	56
3	Cyanic acid, propyl ester	85	C4H7NO	001768-36-1	45
4	2,3-Dimethylsuccinic acid	146	C6H10O4	013545-04-5	45
5	Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	42





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ALS Vial : 13 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 41089

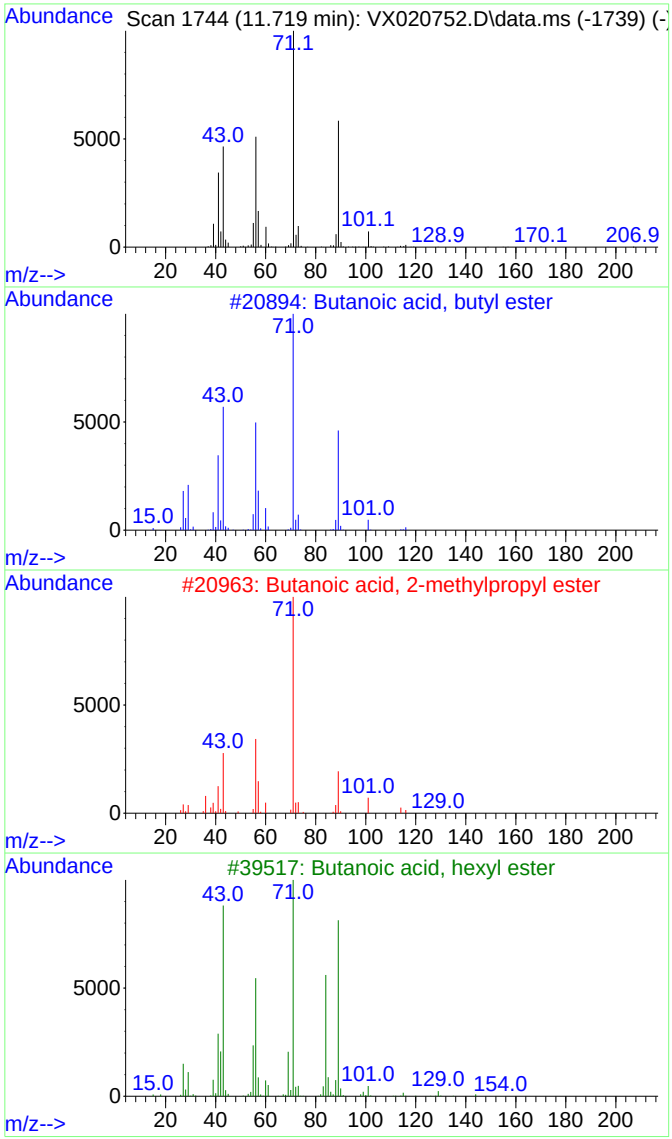
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

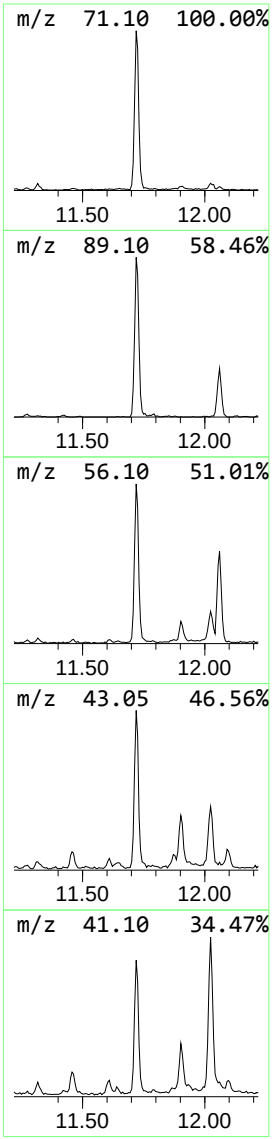
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.719	6.19 ug/l	200785	1,4-Dichlorobenzene-d4	12.060

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	86
2	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64
3	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	45
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	42





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ClientSampleId : 41089

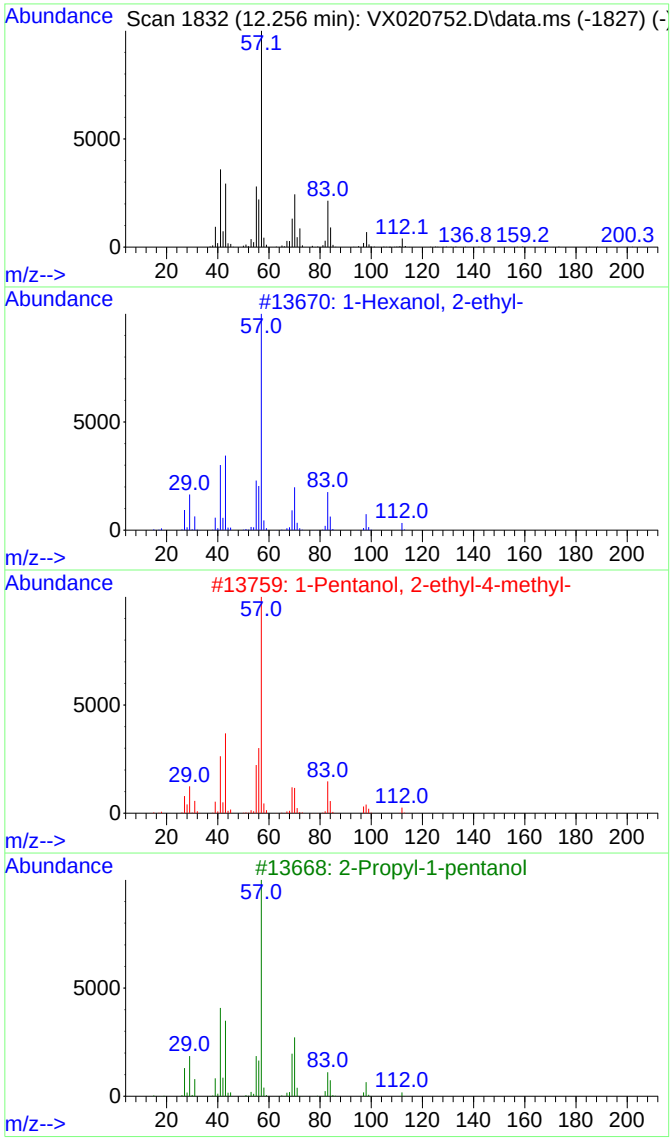
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

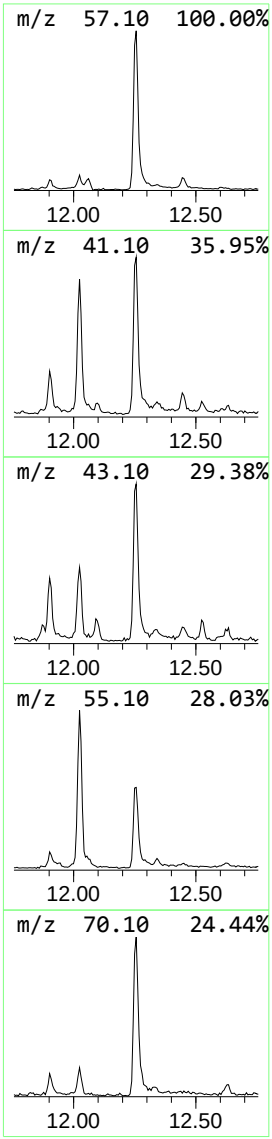
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.256	9.63 ug/l	312155	1,4-Dichlorobenzene-d4	12.060

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
5	3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	47





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane	1.160	25.1	ug/l	520603	1	5.629	1034850	50.0
2-Propanethiol,...	3.757	40.7	ug/l	842181	1	5.629	1034850	50.0
Butanal	4.300	28.8	ug/l	595629	1	5.629	1034850	50.0
1-Butanol	7.263	5.0	ug/l	135751	2	6.830	1354720	50.0
Butanoic acid, ...	11.719	6.2	ug/l	200785	4	12.060	1621160	50.0
1-Hexanol, 2-et...	12.256	9.6	ug/l	312155	4	12.060	1621160	50.0