LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012621\
Data File : VX020753.D
Acq On : 26 Jan 2021 15:07
Operator : JC/SP
Sample : M1189-14
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 41090

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: VX020753.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	22	rVB	759076	662758	15.51%	3.248%
2	1.471	59	63	75	rBV	1182680	1354971	31.72%	6.641%
3	2.416	213	218	232	rVB	42445	79292	1.86%	0.389%
4	2.831	277	286	307	rBV	2242280	4272308	100.00%	20.941%
5	3.014	307	316	329	rVB2	40857	96377	2.26%	0.472%
6	3.757	425	438	450	rBV	187148	522129	12.22%	2.559%
7	4.300	513	527	542	rBV	396677	1081384	25.31%	5.300%
8	4.641	569	583	599	rBV	24862	75167	1.76%	0.368%
9	5.464	706	718	732	rBV	207710	596429	13.96%	2.923%
10	5.629	732	745	758	rVB	350582	985558	23.07%	4.831%
11	6.031	799	811	820	rBV	226119	588106	13.77%	2.883%
12	6.830	929	942	958	rBV	543287	1296842	30.35%	6.356%
13	7.263	1006	1013	1033	rBV	94014	210714	4.93%	1.033%
14	8.695	1241	1248	1254	rBV	1162691	1793285	41.97%	8.790%
15	8.763	1254	1259	1265	rVB	235130	347889	8.14%	1.705%
16	10.092	1469	1477	1489	rBV	1142477	1589366	37.20%	7.790%
17	10.341	1513	1518	1523	rVB	78512	109696	2.57%	0.538%
18	10.683	1569	1574	1579	rBV2	46020	70840	1.66%	0.347%
19	11.122	1640	1646	1651	rBV	915167	1204601	28.20%	5.904%
20	11.171	1651	1654	1658	rVB	56326	68818	1.61%	0.337%
21	11.719	1739	1744	1751	rBV	196479	224662	5.26%	1.101%
22	11.902	1770	1774	1783	rVB	97982	138004	3.23%	0.676%
23	12.024	1786	1794	1796	rBV	148313	200898	4.70%	0.985%
24	12.061	1796	1800	1808	rVB	1224204	1494074	34.97%	7.323%
25	12.256	1826	1832	1842	rBV	502433	736060	17.23%	3.608%
26	13.646	2052	2060	2068	rBV3	42095	71681	1.68%	0.351%
27	13.786	2079	2083	2085	rBV2	49623	62094	1.45%	0.304%
28	13.816	2085	2088	2092	rVV	79077	100936	2.36%	0.495%
29	13.884	2092	2099	2106	rVV	131575	182654	4.28%	0.895%
30	13.951	2106	2110	2117	rVV	143699	184426	4.32%	0.904%

Sum of corrected areas: 20402019

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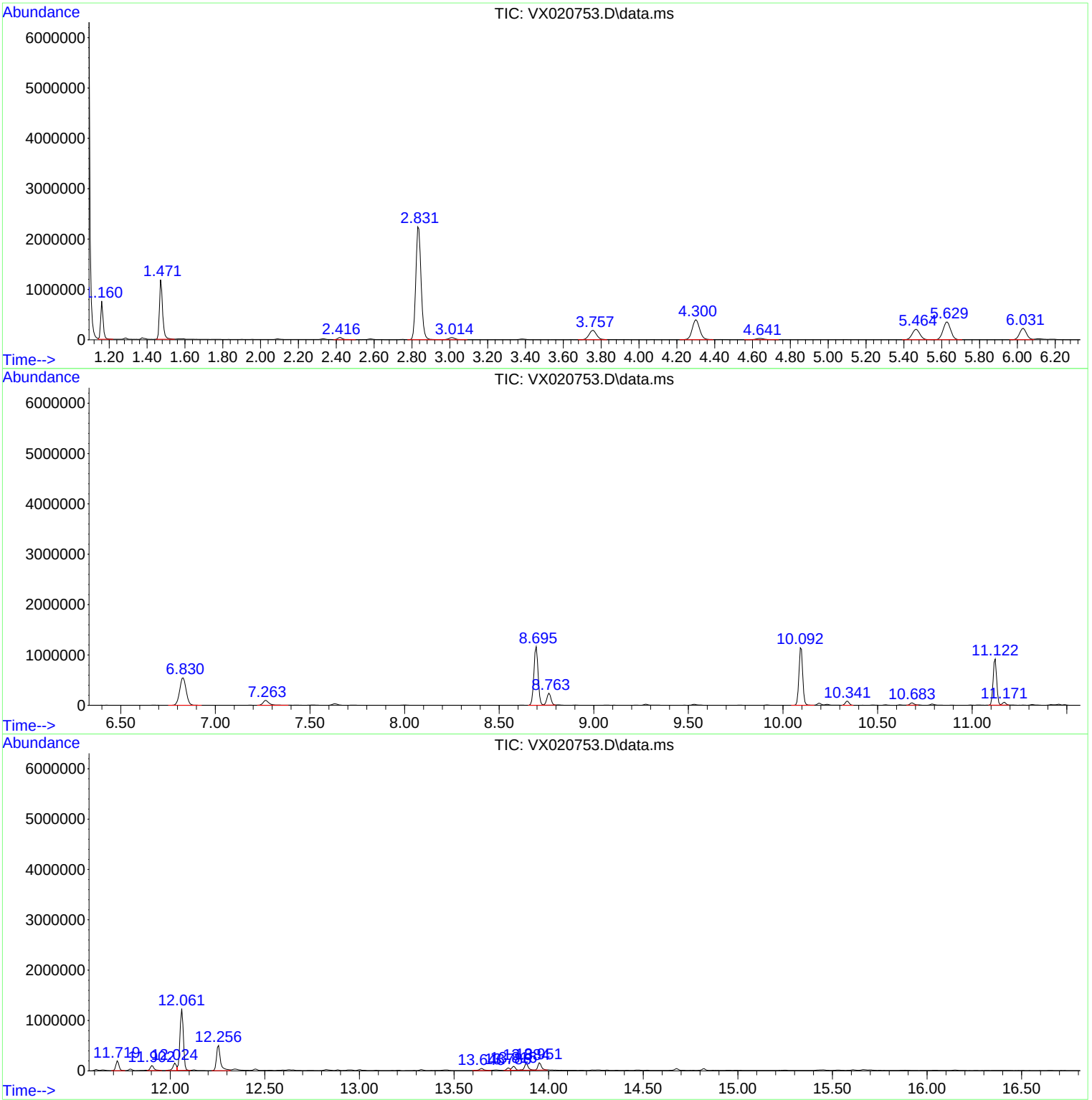
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
41090

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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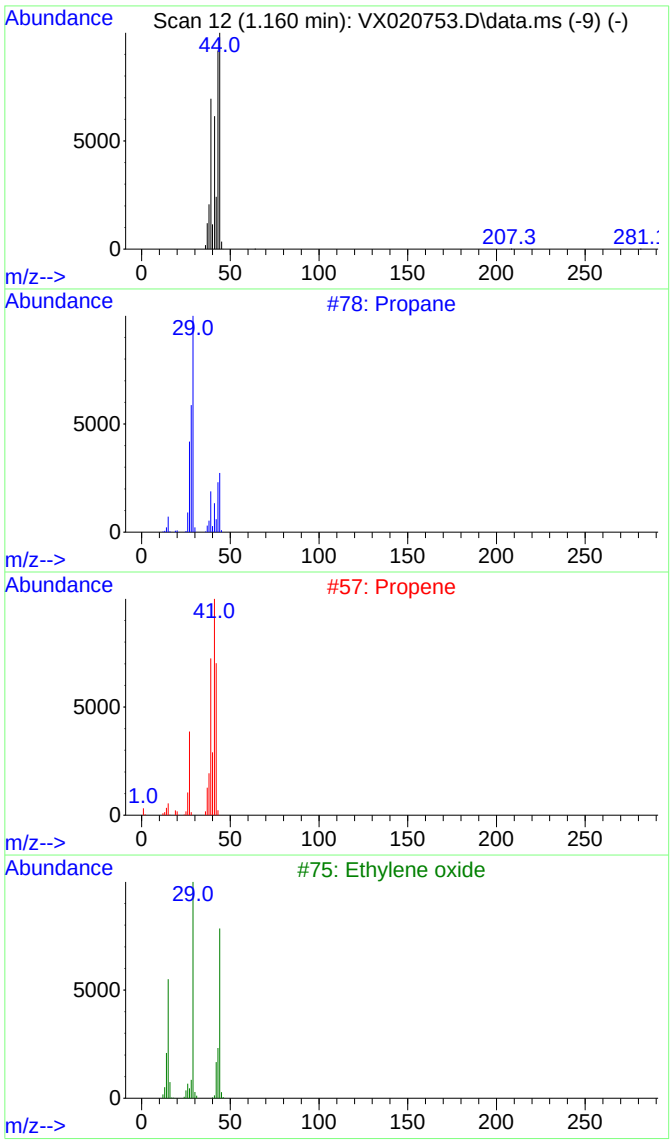
Quant Title : SW846 8260

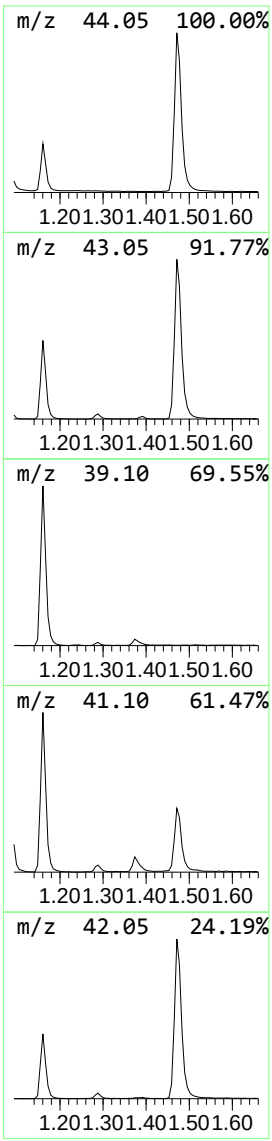
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.160	33.62 ug/l	662758	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	Acetaldehyde	44	C2H4O	000075-07-0	3
5	Ethyne, fluoro-	44	C2HF	002713-09-9	3





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Operator : JC/SP
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Instrument :
MSVOA_X
ClientSampleId :
41090

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

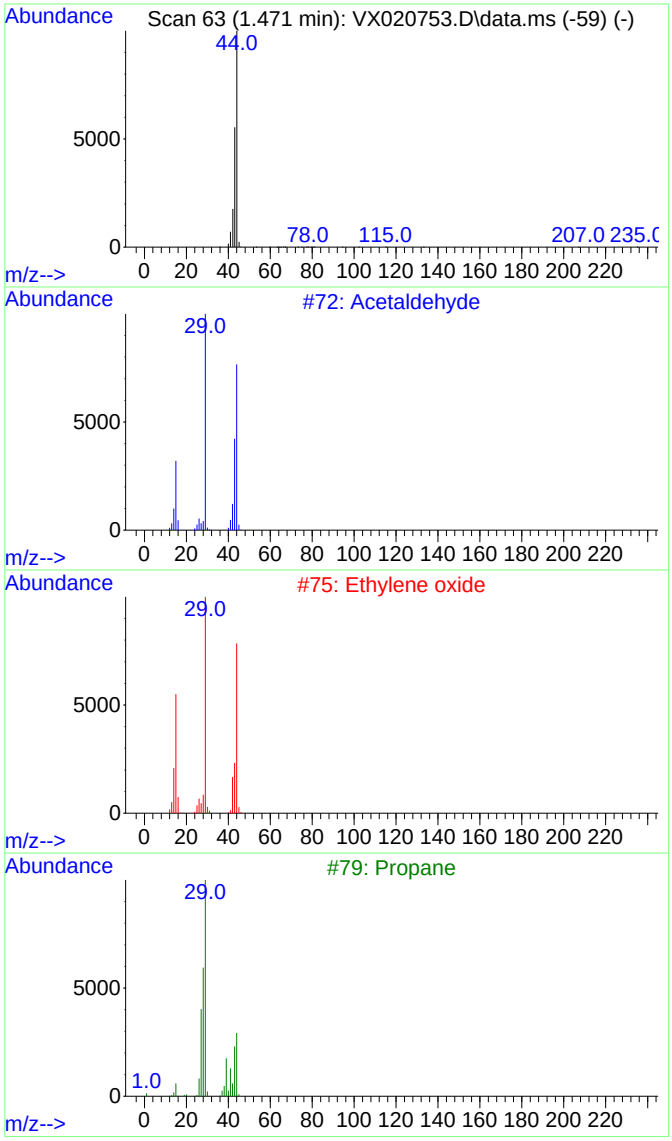
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

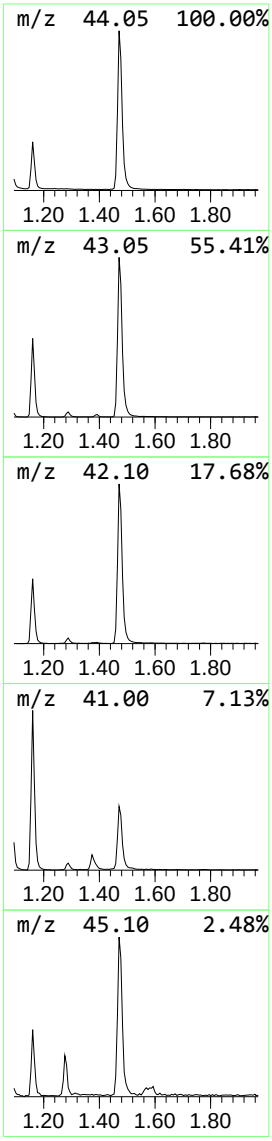
****

Peak Number 2 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.471	68.74 ug/l	1354970	Pentafluorobenzene	5.629

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	56
2	Ethylene oxide	44	C2H4O	000075-21-8	5
3	Propane	44	C3H8	000074-98-6	4
4	Alanine	89	C3H7NO2	000056-41-7	4
5	Ethyne, fluoro-	44	C2HF	002713-09-9	3





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ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 41090

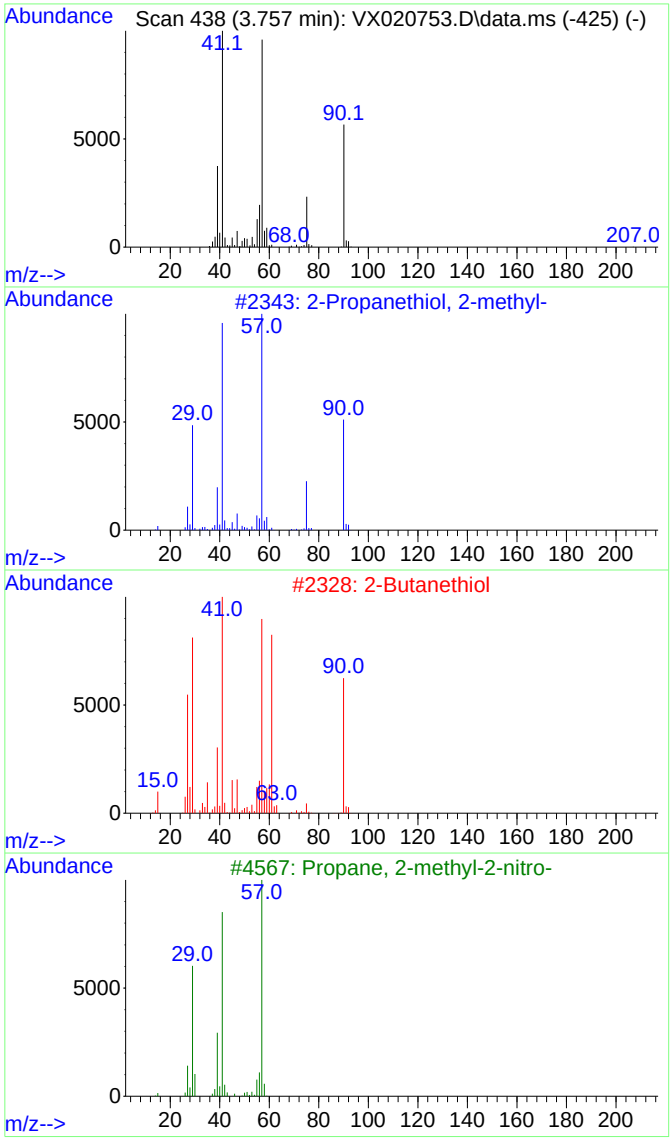
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

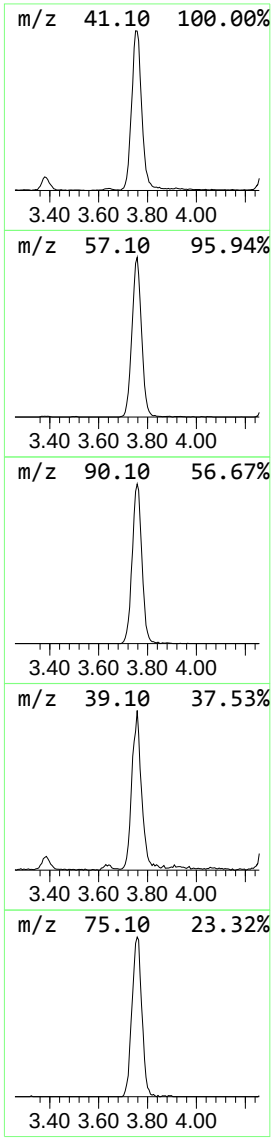
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanethiol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.757	26.49 ug/l	522129	Pentafluorobenzene	5.629

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	87
2	2-Butanethiol	90	C4H10S	000513-53-1	53
3	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	22
4	1-Butene	56	C4H8	000106-98-9	18
5	Butane, 2-nitro-	103	C4H9NO2	000600-24-8	17





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Instrument :
MSVOA_X
ClientSampleId :
41090

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

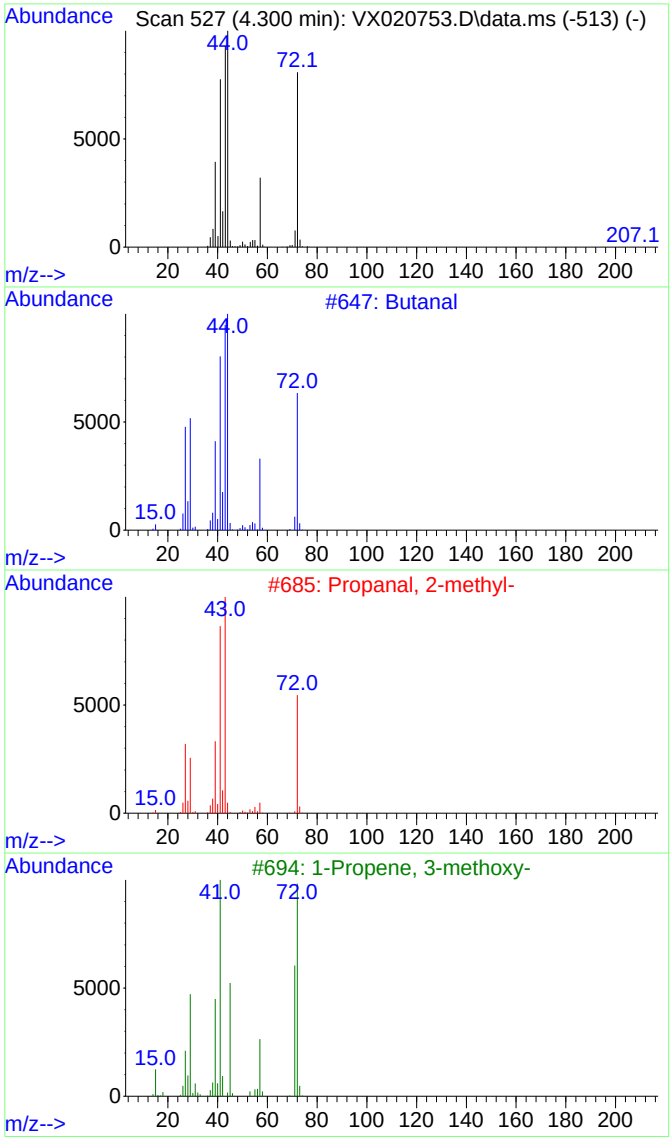
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

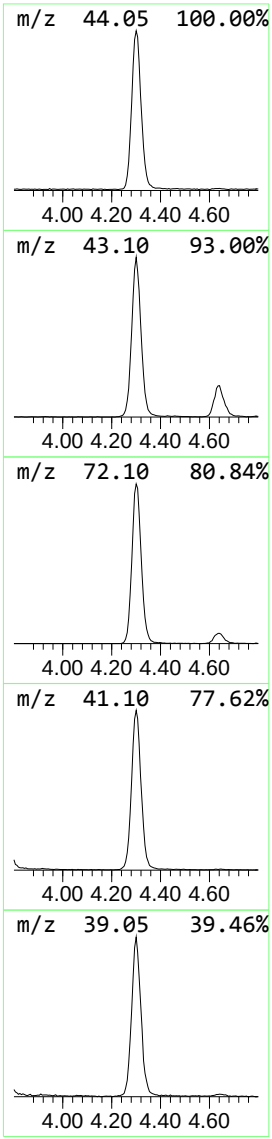
****

Peak Number 4 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.300	54.86 ug/l	1081380	Pentafluorobenzene	5.629

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	46
3	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43
4	O-Methylisourea	74	C2H6N2O	002440-60-0	37
5	Isobutylene epoxide	72	C4H8O	000558-30-5	27





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ALS Vial : 14 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 41090

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

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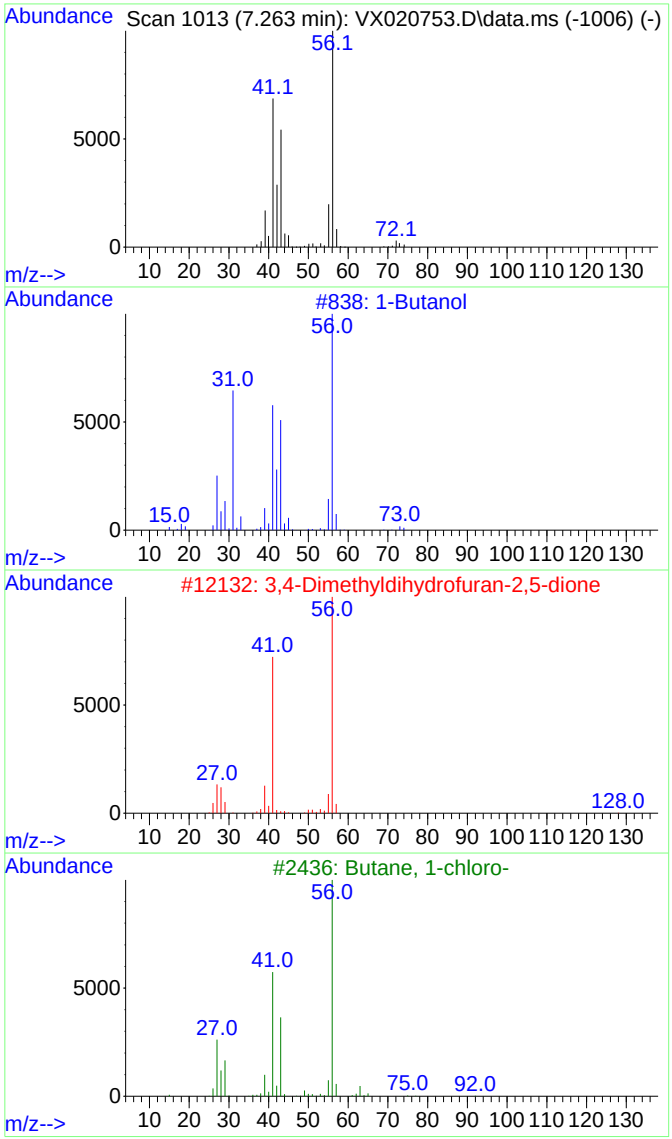
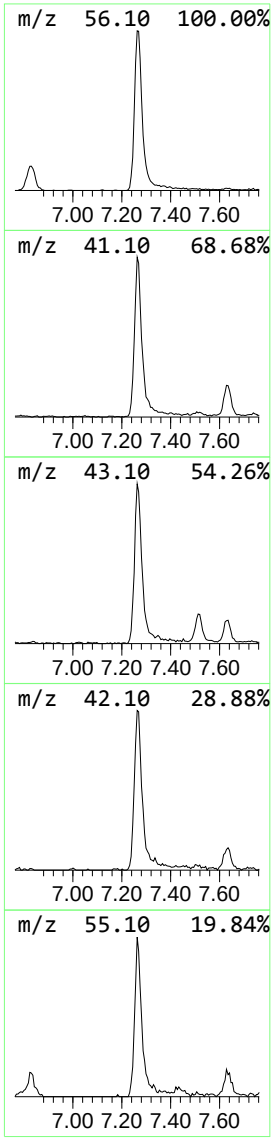
****

Peak Number 5 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.263	8.12 ug/l	210714	1,4-Difluorobenzene	6.830

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	91
2	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	42
3	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	36
4	Propanenitrile, 2-hydroxy-	71	C3H5NO	000078-97-7	9
5	Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	9





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Instrument : MSVOA_X
ClientSampleId : 41090

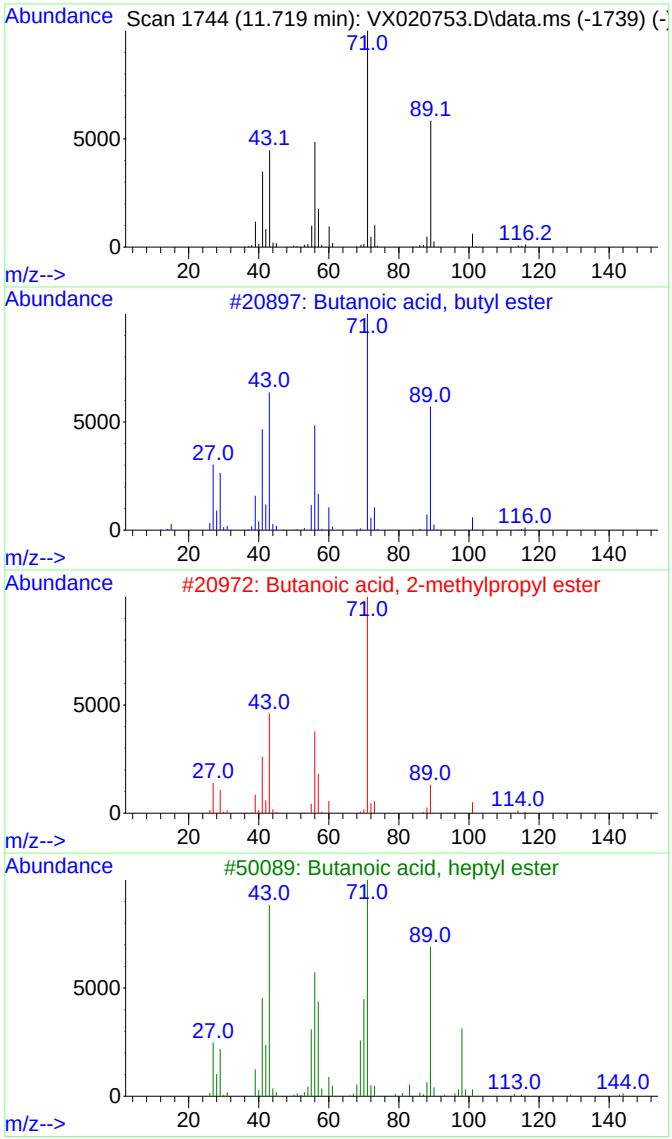
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012521W.M
Quant Title : SW846 8260

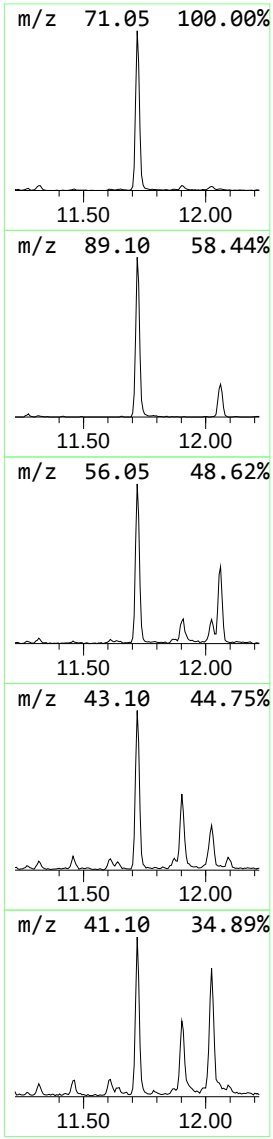
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Butanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.719	7.52 ug/l	224662	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
3	Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	64
4	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
5	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	59





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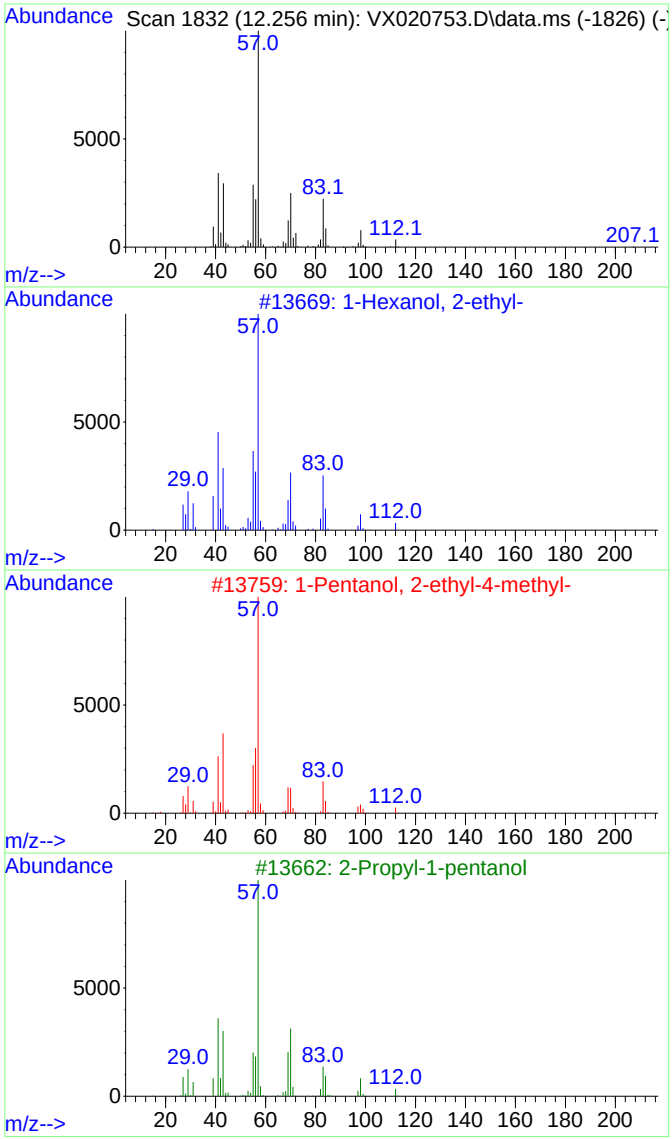
Quant Title : SW846 8260

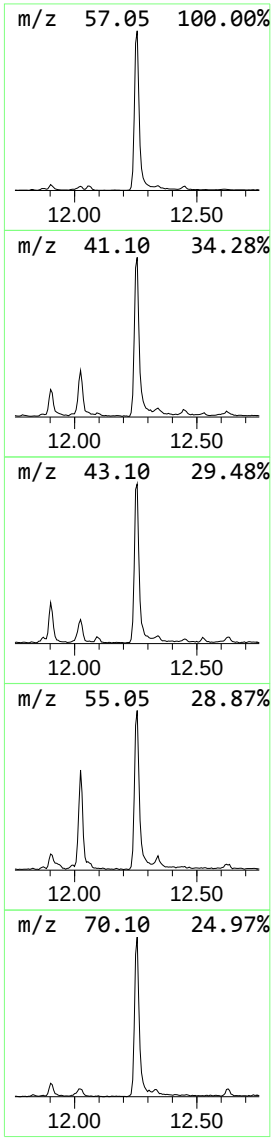
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.256	24.63 ug/l	736060	1,4-Dichlorobenzene-d4	12.061

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	59
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
5	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	47





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ClientSampleId :
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TIC Library : C:\DATABASE\NIST11.L
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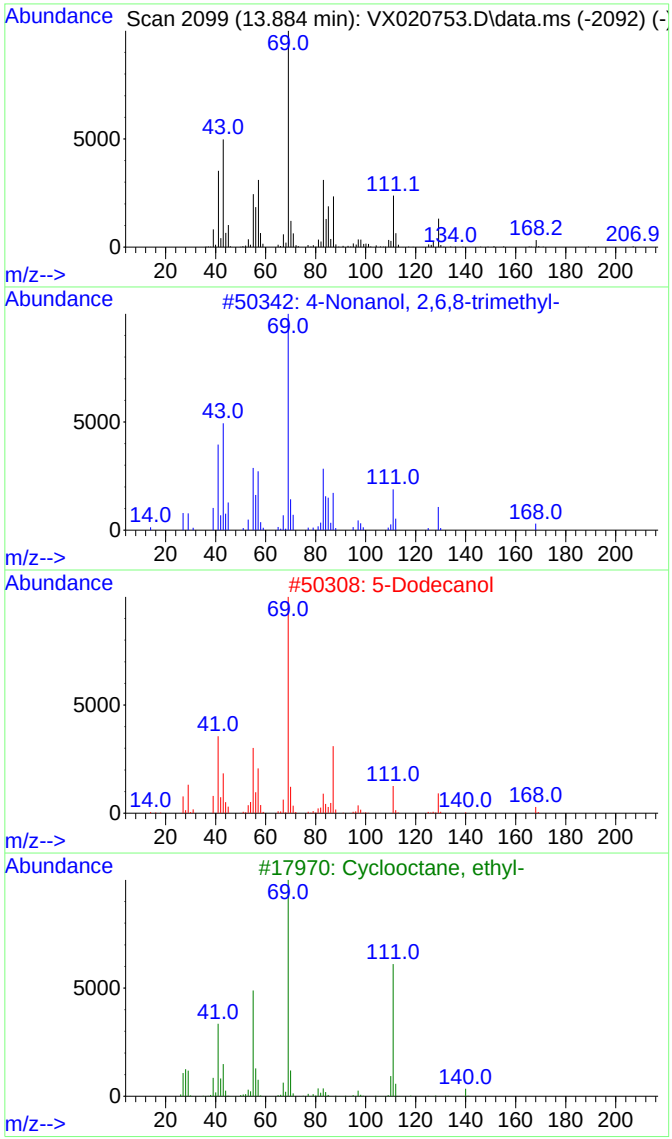
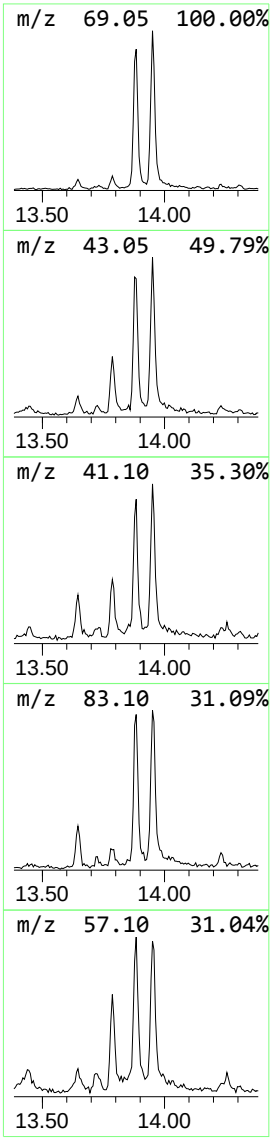
****
Peak Number 8 4-Nonanol, 2,6,8-trimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.884	6.11 ug/l	182654	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Nonanol, 2,6,8-trimethyl-	186	C12H26O	000123-17-1	80
2	5-Dodecanol	186	C12H26O	010203-33-5	59
3	Cyclooctane, ethyl-	140	C10H20	013152-02-8	47
4	1,2-Hexanediol	118	C6H14O2	006920-22-5	43
5	Cyclooctane, (1-methylpropyl)-	168	C12H24	016538-89-9	38





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

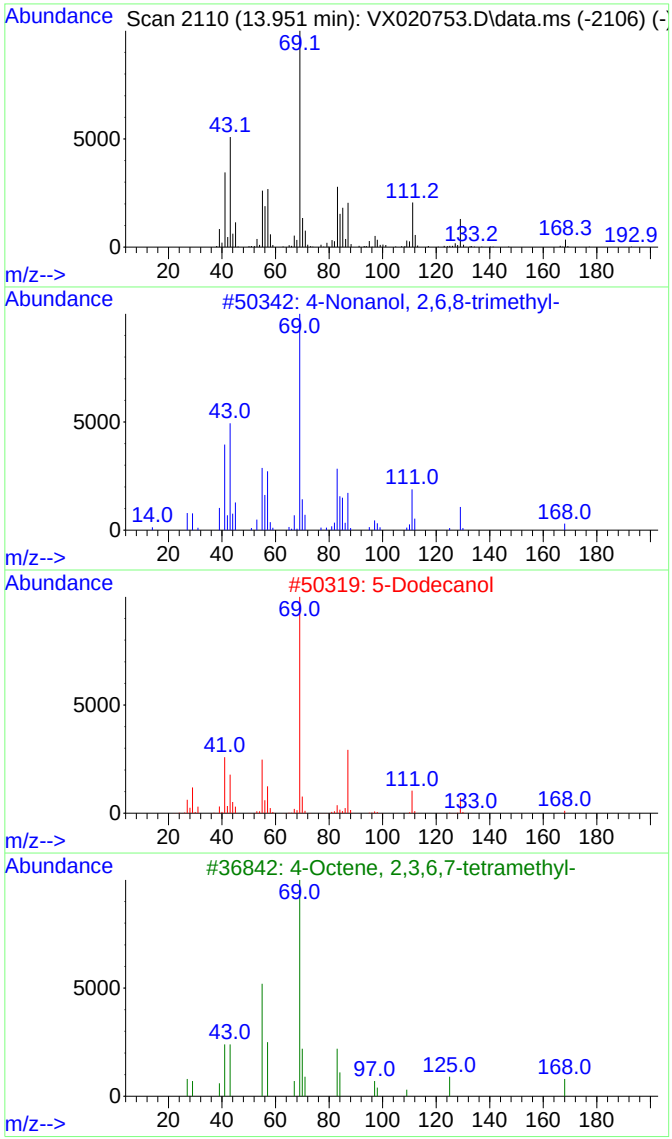
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

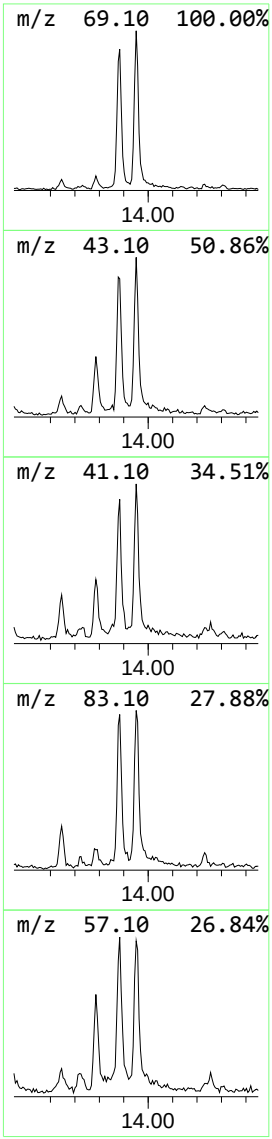
****

Peak Number 9 5-Dodecanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.951	6.17 ug/l	184426	1,4-Dichlorobenzene-d4	12.061

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Nonanol, 2,6,8-trimethyl-	186	C12H26O	000123-17-1	91
2	5-Dodecanol	186	C12H26O	010203-33-5	53
3	4-Octene, 2,3,6,7-tetramethyl-	168	C12H24	063830-66-0	47
4	Cyclohexane, (1,2-dimethylbutyl)-	168	C12H24	061142-37-8	45
5	3-Heptanol, 2-methyl-	130	C8H18O	018720-62-2	43





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane	1.160	33.6	ug/l	662758	1	5.629	985558	50.0
Acetaldehyde	1.471	68.7	ug/l	1354970	1	5.629	985558	50.0
2-Propanethiol,...	3.757	26.5	ug/l	522129	1	5.629	985558	50.0
Butanal	4.300	54.9	ug/l	1081380	1	5.629	985558	50.0
1-Butanol	7.263	8.1	ug/l	210714	2	6.830	1296840	50.0
Butanoic acid, ...	11.719	7.5	ug/l	224662	4	12.061	1494070	50.0
1-Hexanol, 2-et...	12.256	24.6	ug/l	736060	4	12.061	1494070	50.0
4-Nonanol, 2,6,...	13.884	6.1	ug/l	182654	4	12.061	1494070	50.0
5-Dodecanol	13.951	6.2	ug/l	184426	4	12.061	1494070	50.0