LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021111.D
Acq On : 09 Mar 2021 16:11
Operator : JC/MD
Sample : M1578-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : COMP-2

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\82X022421W.M
Title : SW846 8260

Signal : TIC: VX021111.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.164	9	13	21	rBV	156453	148147	11.76%	1.739%
2	1.393	47	52	58	rVB2	14277	18698	1.48%	0.219%
3	2.417	220	226	239	rVB	37154	63141	5.01%	0.741%
4	2.570	246	252	262	rVB	15505	29483	2.34%	0.346%
5	3.011	316	327	334	rBV6	5834	15656	1.24%	0.184%
6	3.758	443	454	467	rBV2	25082	72671	5.77%	0.853%
7	4.299	536	546	565	rBV	43323	124058	9.85%	1.456%
8	5.464	732	744	759	rBV	138612	397540	31.57%	4.665%
9	5.629	759	772	791	rVV	217040	608304	48.31%	7.139%
10	6.035	828	841	849	rBV	150078	393432	31.24%	4.617%
11	6.117	849	855	863	rVB	17700	46566	3.70%	0.546%
12	6.829	965	976	1000	rBV	366558	890694	70.73%	10.453%
13	7.265	1043	1050	1060	rBV2	6611	17589	1.40%	0.206%
14	7.635	1107	1113	1120	rBV	7685	13518	1.07%	0.159%
15	8.335	1225	1232	1237	rBV2	8815	16279	1.29%	0.191%
16	8.694	1286	1293	1300	rBV	806748	1259231	100.00%	14.778%
17	8.765	1300	1305	1311	rVB	71379	112980	8.97%	1.326%
18	10.094	1524	1531	1543	rBV	818135	1129928	89.73%	13.260%
19	10.194	1543	1548	1551	rVV	17017	26335	2.09%	0.309%
20	10.236	1551	1555	1561	rVB	20159	28196	2.24%	0.331%
21	10.341	1567	1573	1579	rBV	78496	108371	8.61%	1.272%
22	10.683	1626	1631	1642	rVB	58478	82475	6.55%	0.968%
23	10.789	1644	1649	1659	rBV	10411	17805	1.41%	0.209%
24	11.118	1699	1705	1711	rBV	651880	863586	68.58%	10.135%
25	11.171	1711	1714	1719	rVB2	14289	20059	1.59%	0.235%
26	11.418	1752	1756	1759	rBV	9977	14115	1.12%	0.166%
27	11.606	1783	1788	1793	rBV	77328	103106	8.19%	1.210%
28	11.642	1793	1794	1802	rVV3	10764	15962	1.27%	0.187%
29	11.724	1802	1808	1815	rVV	96649	123692	9.82%	1.452%
30	11.795	1815	1820	1824	rVV	19989	26792	2.13%	0.314%
31	11.865	1828	1832	1835	rVV	12218	17191	1.37%	0.202%
32	11.906	1835	1839	1846	rVV	34342	55465	4.40%	0.651%
33	11.989	1846	1853	1856	rVV	21339	36950	2.93%	0.434%
34	12.024	1856	1859	1861	rVV	38722	50970	4.05%	0.598%
35	12.059	1861	1865	1873	rVV	834995	1077094	85.54%	12.640%
36	12.124	1873	1876	1882	rVB	10880	15267	1.21%	0.179%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021111.D
Acq On : 09 Mar 2021 16:11
Operator : JC/MD
Sample : M1578-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : COMP-2

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\82X022421W.M
Title : SW846 8260

37	12.253	1893	1898	1910	rBV	106369	193416	15.36%	2.270%
38	12.342	1910	1913	1924	rVV7	13466	33410	2.65%	0.392%
39	12.448	1927	1931	1936	rVB	16502	22891	1.82%	0.269%
40	12.889	2002	2006	2013	rVB2	13884	20151	1.60%	0.236%
41	13.030	2027	2030	2035	rVB	13657	16938	1.35%	0.199%
42	13.648	2124	2135	2142	rBV7	9114	18953	1.51%	0.222%
43	13.771	2152	2156	2159	rBV2	11727	15317	1.22%	0.180%
44	13.812	2159	2163	2170	rVV	58956	77607	6.16%	0.911%
45	13.883	2170	2175	2183	rVB4	12577	18789	1.49%	0.220%
46	13.954	2183	2187	2194	rBV2	12292	18237	1.45%	0.214%
47	14.677	2302	2310	2314	rBV	10393	14800	1.18%	0.174%
48	16.025	2533	2539	2548	rBV5	7500	14710	1.17%	0.173%
49	16.148	2555	2560	2567	rVB3	8556	14640	1.16%	0.172%

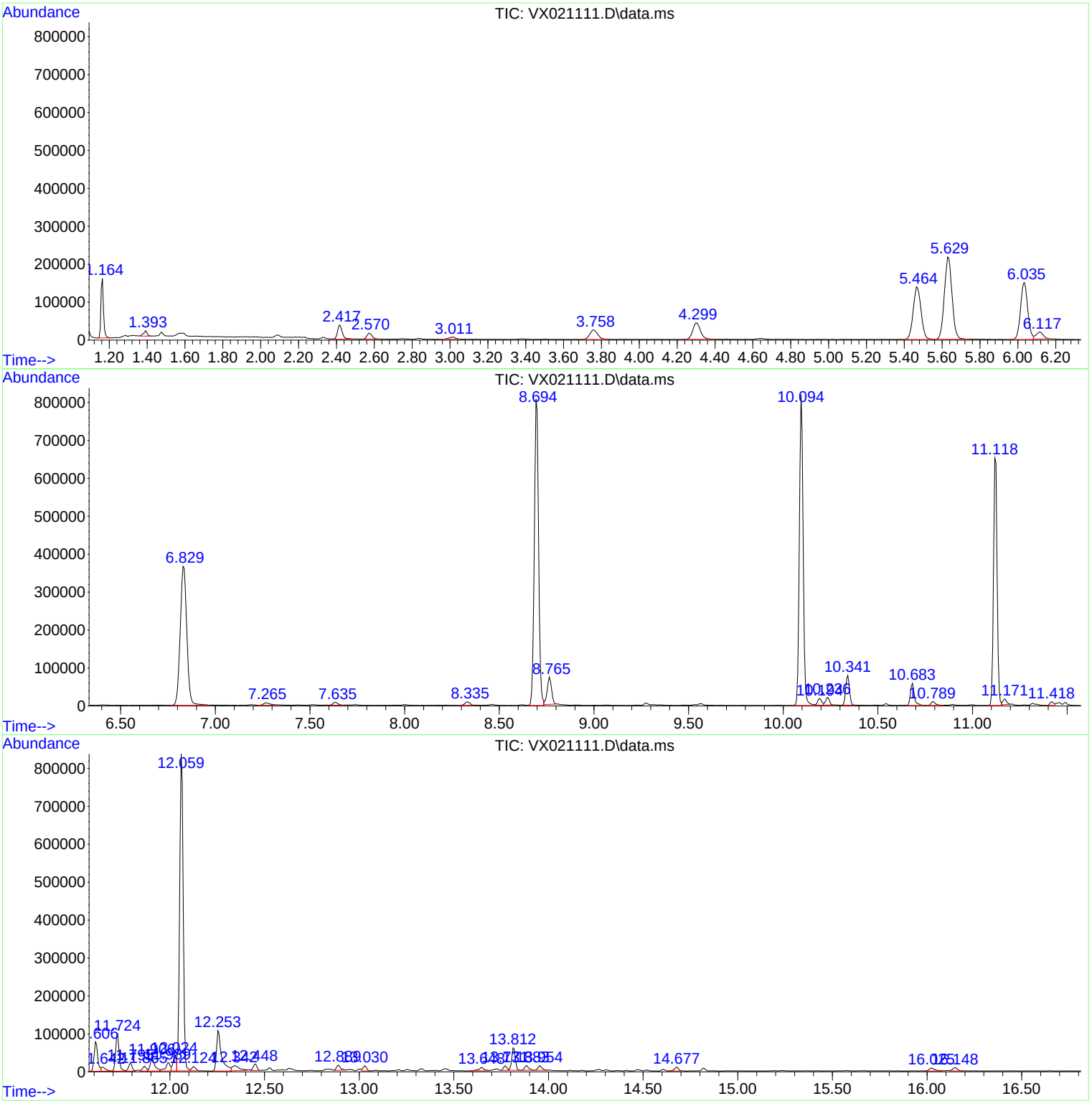
Sum of corrected areas: 8521205

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021111.D
Acq On : 09 Mar 2021 16:11
Operator : JC/MD
Sample : M1578-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021111.D
Acq On : 09 Mar 2021 16:11
Operator : JC/MD
Sample : M1578-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

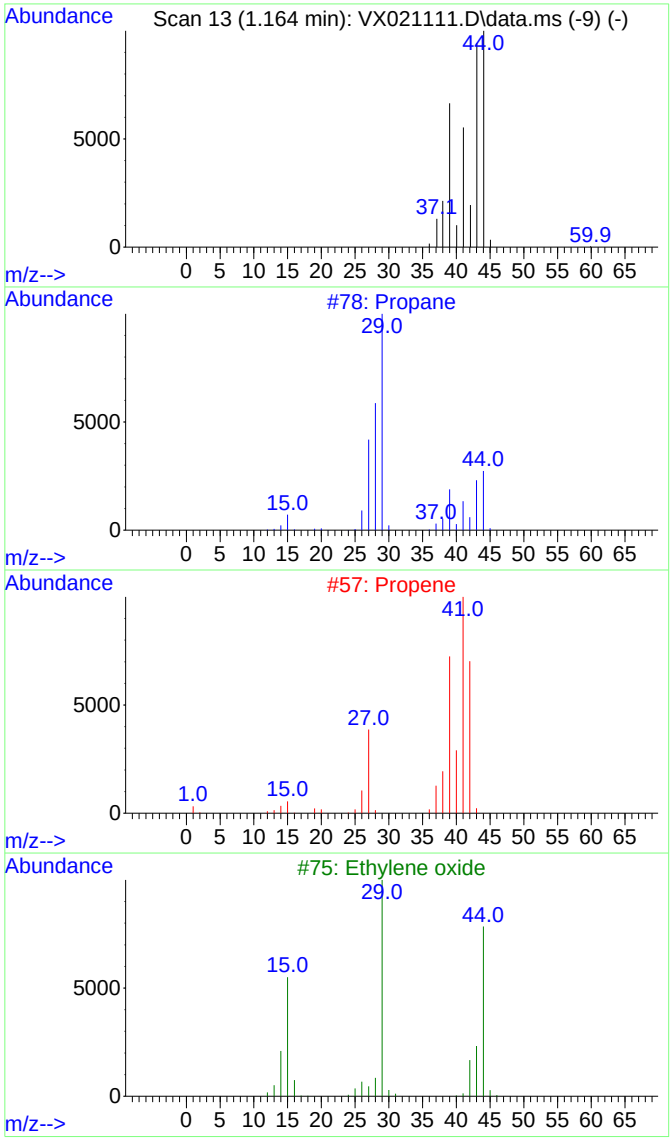
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

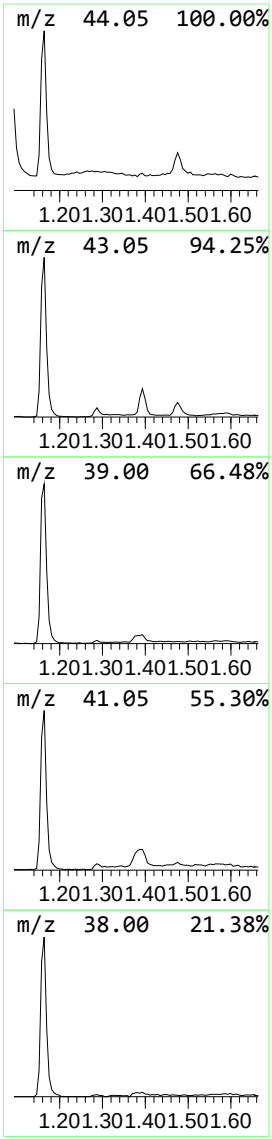
****

Peak Number 1 Propane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.164	12.18 ug/l	148147	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	5
5	Ethyne, fluoro-	44	C2HF	002713-09-9	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021111.D
Acq On : 09 Mar 2021 16:11
Operator : JC/MD
Sample : M1578-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-2

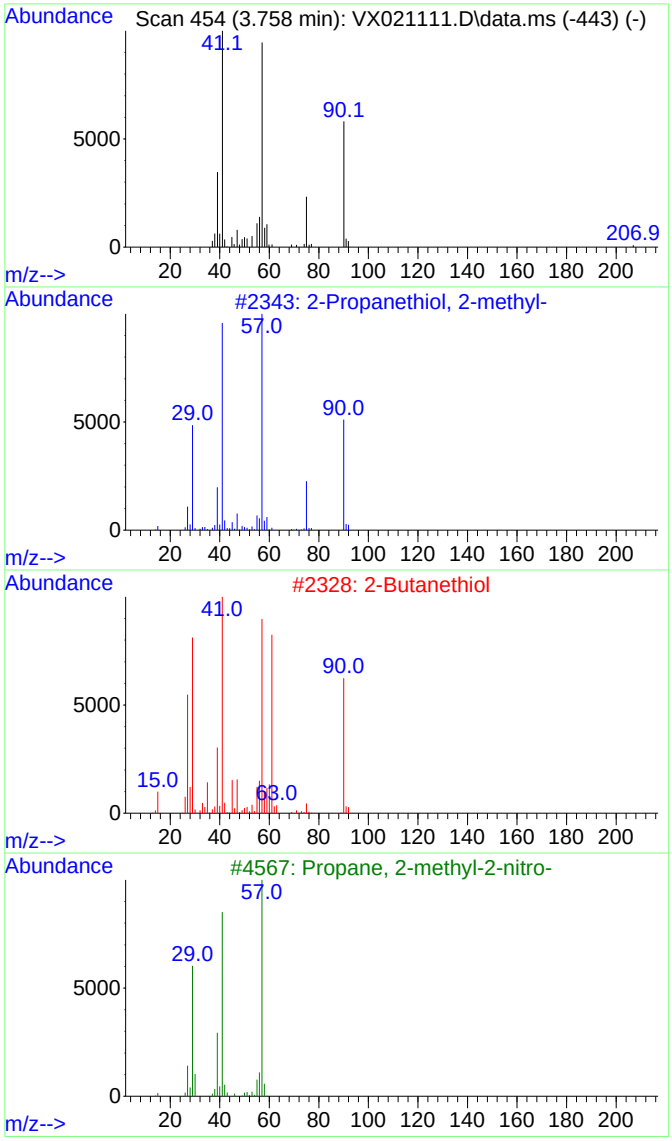
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

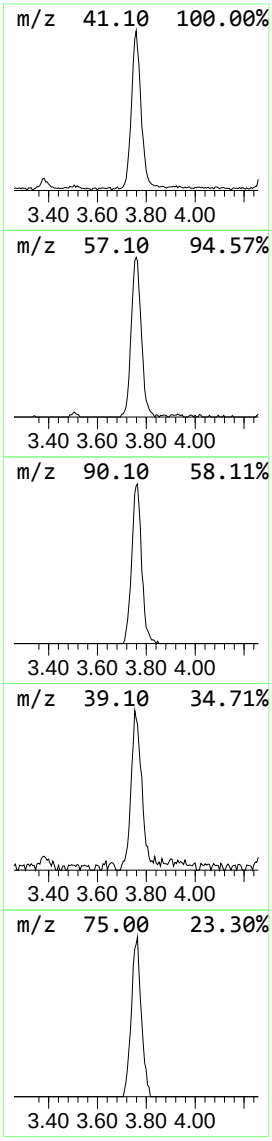
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.758	5.97 ug/l	72671	Pentafluorobenzene	5.629

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	90
2	2-Butanethiol	90	C4H10S	000513-53-1	59
3	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	22
4	Thiourea, methyl-	90	C2H6N2S	000598-52-7	22
5	Ethynyl tert-butyl sulfoxide	130	C6H10OS	041463-34-7	17





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021111.D
Acq On : 09 Mar 2021 16:11
Operator : JC/MD
Sample : M1578-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

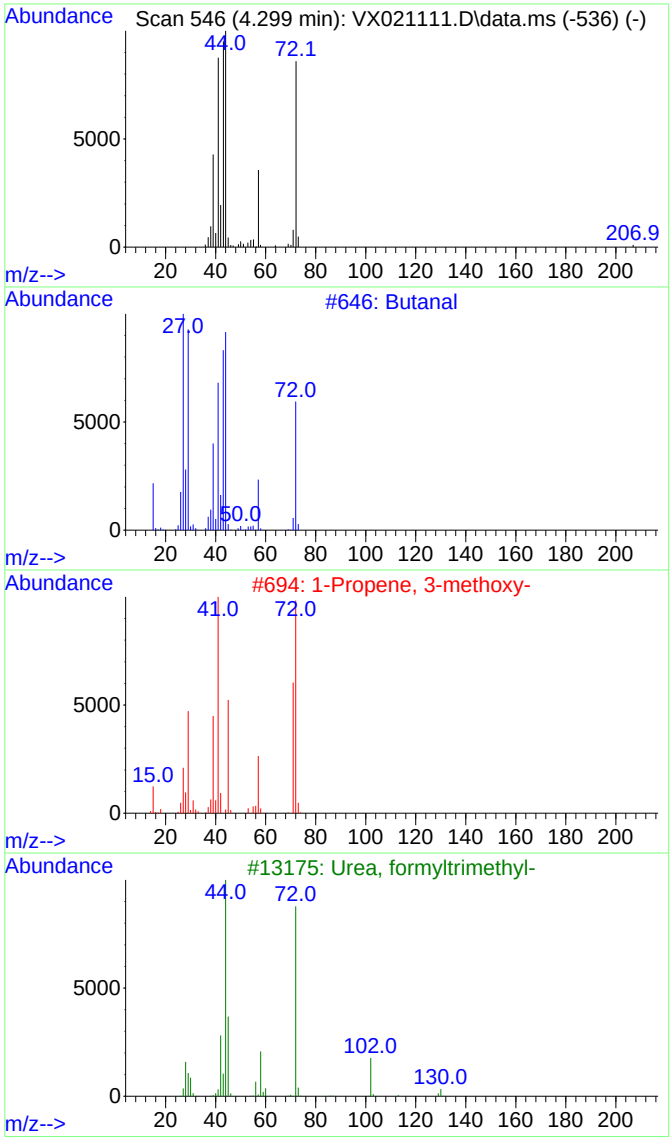
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

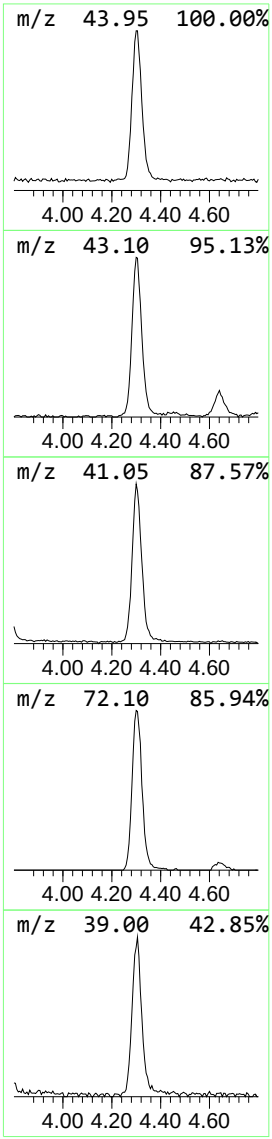
****

Peak Number 3 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.299	10.20 ug/l	124058	Pentafluorobenzene	5.629

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	43
3	Urea, formyltrimethyl-	130	C5H10N2O2	1000151-45-7	40
4	Ethene, ethoxy-	72	C4H8O	000109-92-2	40
5	Propanal, 2-methyl-	72	C4H8O	000078-84-2	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021111.D
Acq On : 09 Mar 2021 16:11
Operator : JC/MD
Sample : M1578-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-2

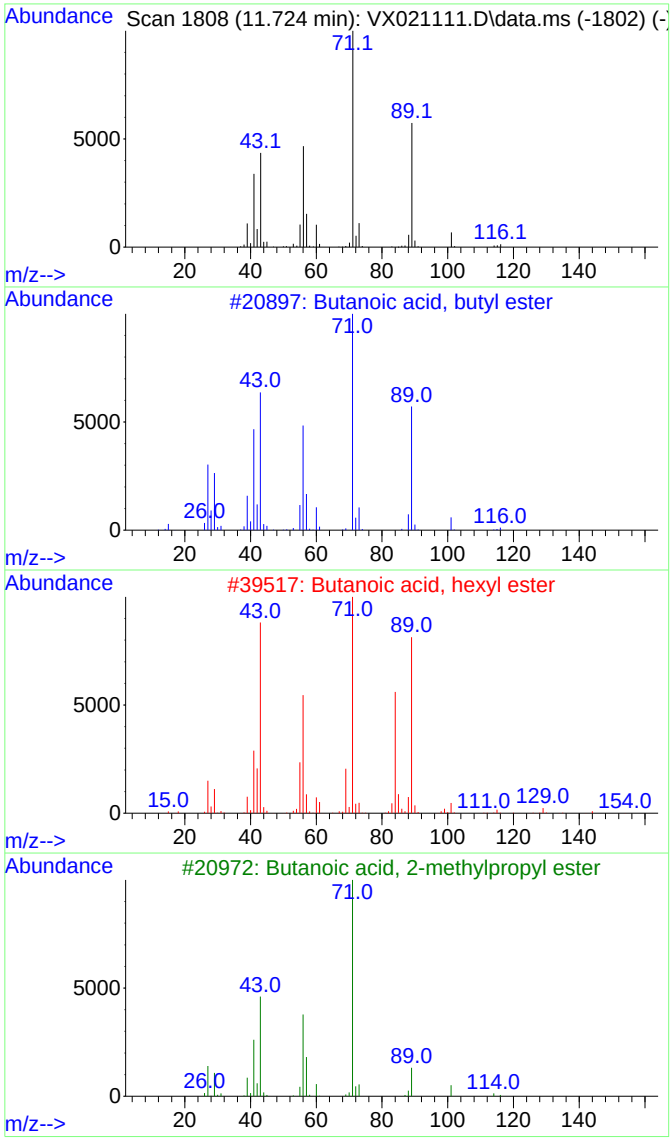
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

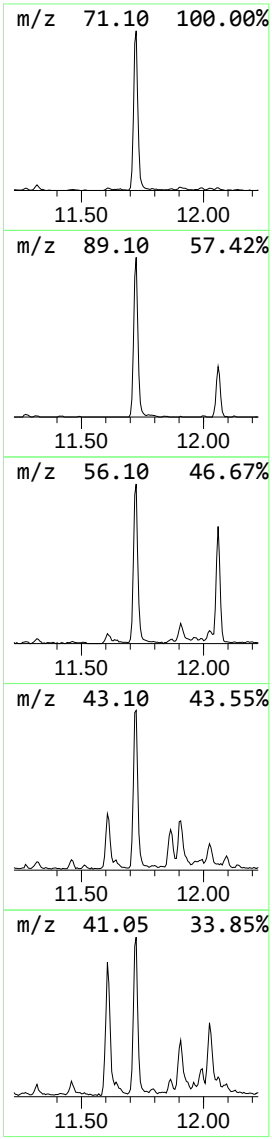
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.724	5.74 ug/l	123692	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
3	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	59
4	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	59
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021111.D
Acq On : 09 Mar 2021 16:11
Operator : JC/MD
Sample : M1578-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
Quant Title : SW846 8260

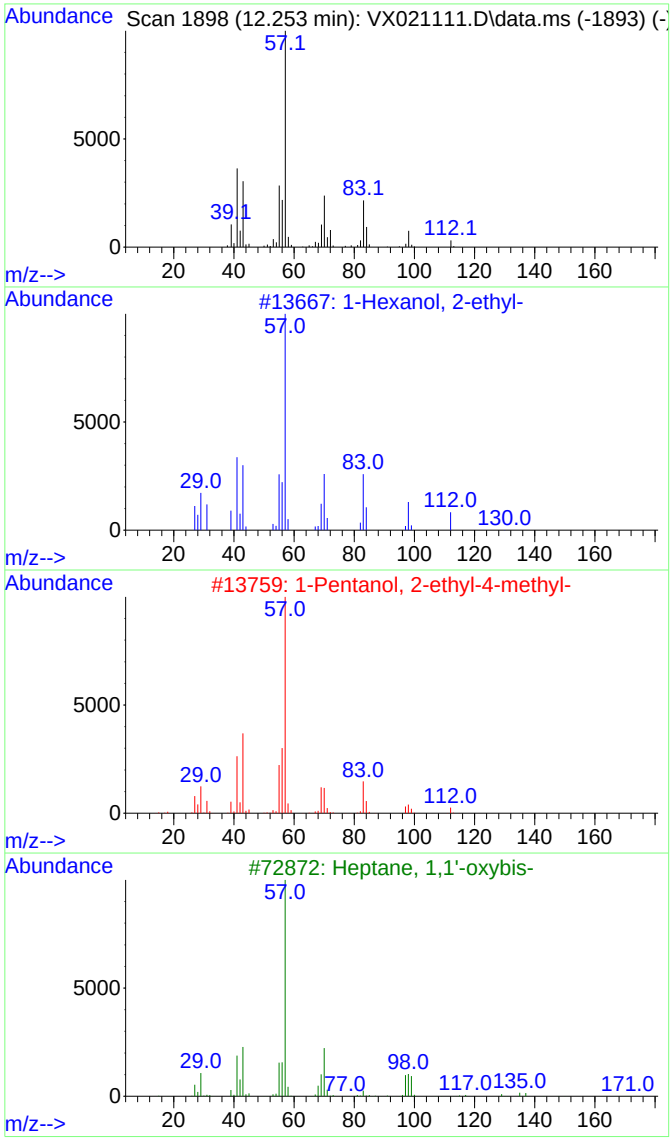
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

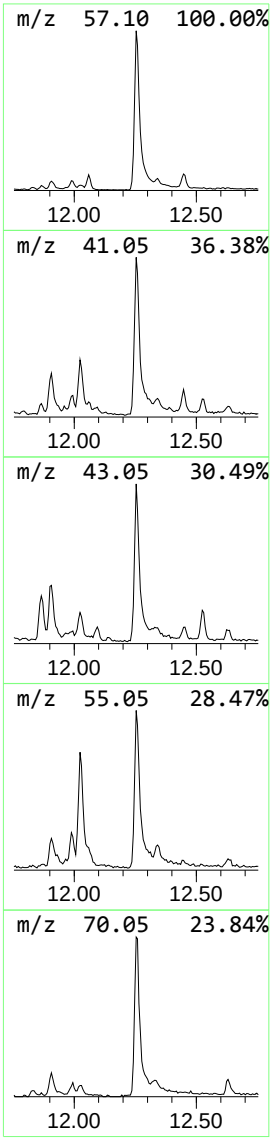
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.253	8.98 ug/l	193416	1,4-Dichlorobenzene-d4	12.059

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX030921\
Data File : VX021111.D
Acq On : 09 Mar 2021 16:11
Operator : JC/MD
Sample : M1578-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : COMP-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X022421W.M
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	1.164	12.2	ug/l	148147	1	5.629	608304	50.0
2-Propanethiol,...	3.758	6.0	ug/l	72671	1	5.629	608304	50.0
Butanal	4.299	10.2	ug/l	124058	1	5.629	608304	50.0
Butanoic acid, ...	11.724	5.7	ug/l	123692	4	12.059	1077090	50.0
1-Hexanol, 2-et...	12.253	9.0	ug/l	193416	4	12.059	1077090	50.0