LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112322\
Data File : VX033046.D
Acq On : 24 Nov 2022 07:59
Operator : JC/MD
Sample : N5741-20
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-40

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\82X112222W.M
Title : SW846 8260

Signal : TIC: VX033046.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	41	rBV	306992	438454	29.53%	7.190%
2	1.368	42	46	52	rVB2	8635	14917	1.00%	0.245%
3	2.995	301	313	325	rVV	46173	190833	12.85%	3.129%
4	3.111	325	332	345	rVB2	51167	121968	8.22%	2.000%
5	3.763	428	439	448	rBV	26795	72549	4.89%	1.190%
6	4.312	519	529	540	rBV2	15145	44866	3.02%	0.736%
7	5.385	694	705	716	rBV2	64582	190693	12.84%	3.127%
8	5.550	723	732	749	rVB	134583	384589	25.90%	6.307%
9	5.958	788	799	804	rBV	69380	181165	12.20%	2.971%
10	6.037	804	812	826	rVB	562727	1484621	100.00%	24.346%
11	6.251	832	847	859	rBV4	7064	28277	1.90%	0.464%
12	6.763	921	931	945	rBV	206345	493480	33.24%	8.093%
13	8.427	1198	1204	1210	rBV	21327	37994	2.56%	0.623%
14	8.647	1234	1240	1248	rBV	322025	506848	34.14%	8.312%
15	8.958	1282	1291	1298	rBV	39165	63204	4.26%	1.036%
16	9.049	1298	1306	1313	rBV	50848	77839	5.24%	1.276%
17	9.458	1365	1373	1386	rBV	42412	74188	5.00%	1.217%
18	9.945	1448	1453	1460	rBV	16015	23434	1.58%	0.384%
19	10.055	1465	1471	1484	rVB	439498	589301	39.69%	9.664%
20	10.640	1563	1567	1573	rVB	12911	17416	1.17%	0.286%
21	10.963	1614	1620	1624	rBV	12406	17456	1.18%	0.286%
22	11.079	1634	1639	1650	rBV	276836	355476	23.94%	5.829%
23	11.616	1723	1727	1735	rVB	15739	20436	1.38%	0.335%
24	11.750	1746	1749	1756	rVB	12911	16757	1.13%	0.275%
25	12.024	1788	1794	1800	rBV	421699	545385	36.74%	8.944%
26	12.085	1800	1804	1811	rVB	17457	22177	1.49%	0.364%
27	12.244	1822	1830	1835	rBV	29707	38797	2.61%	0.636%
28	12.701	1901	1905	1913	rVB2	17006	25830	1.74%	0.424%
29	13.292	1997	2002	2007	rVB2	13793	18948	1.28%	0.311%

Sum of corrected areas: 6097898

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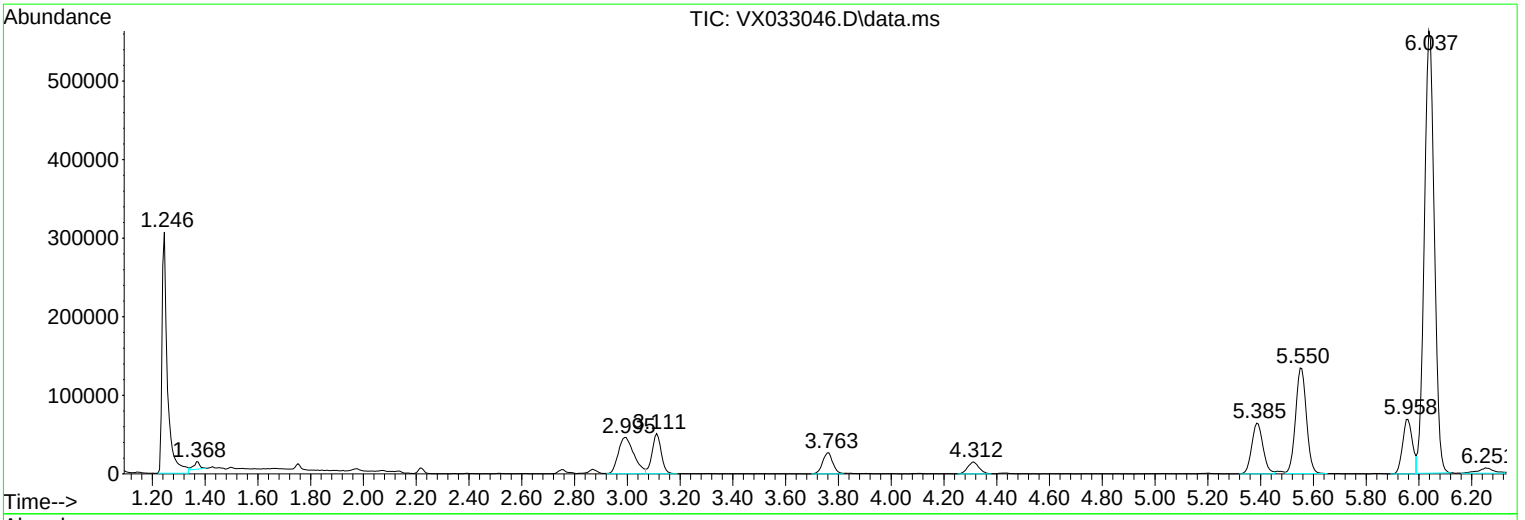
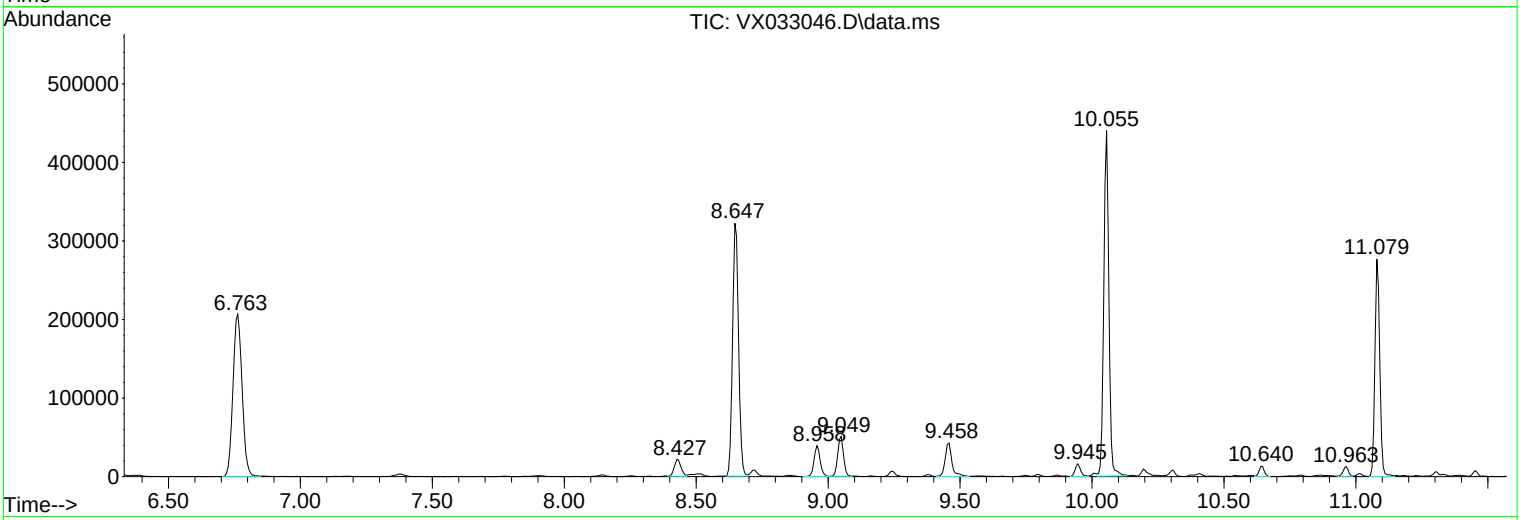
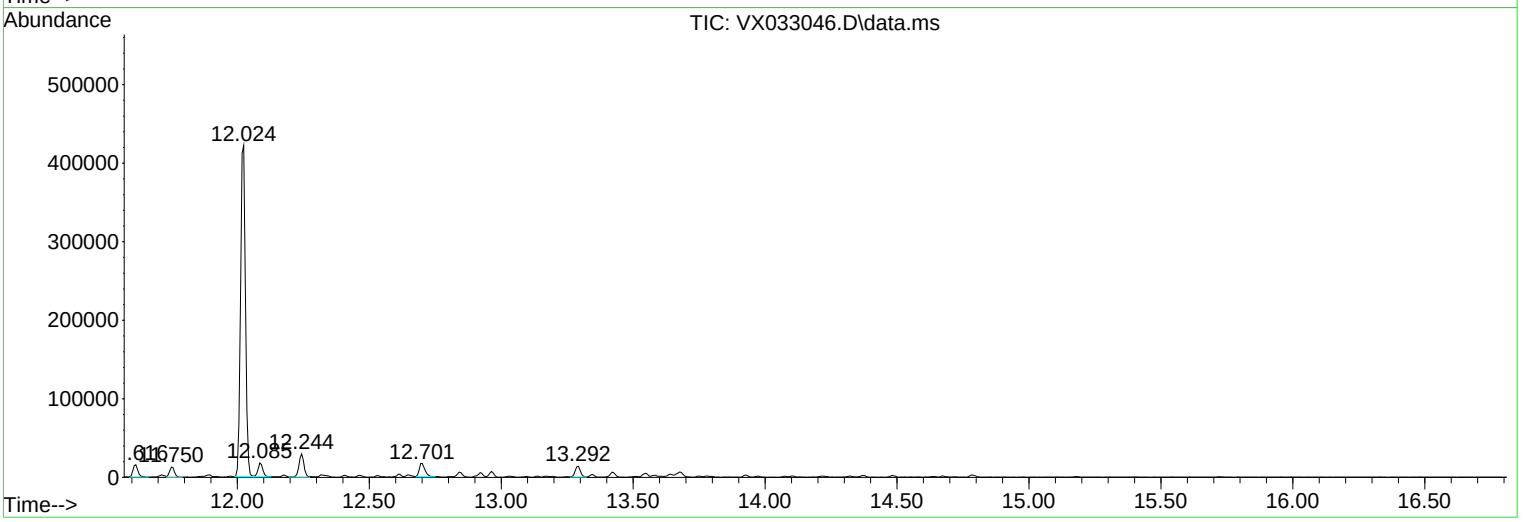
ClientSampleId :
MW-40

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

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







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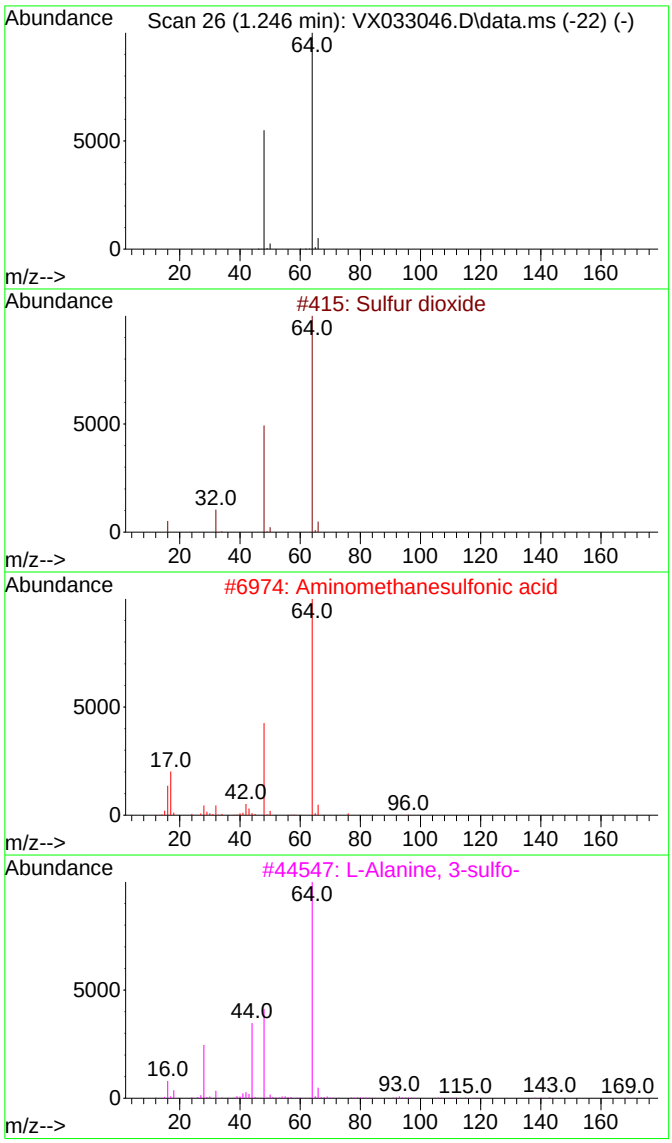
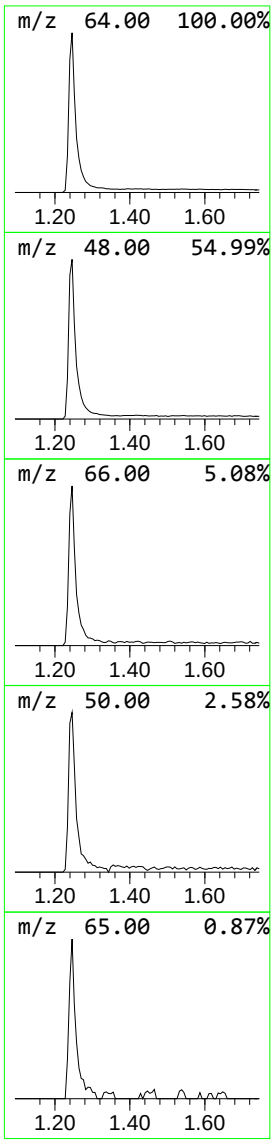
****
Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	57.00 ug/l	438454	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	3





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ClientSampleId :
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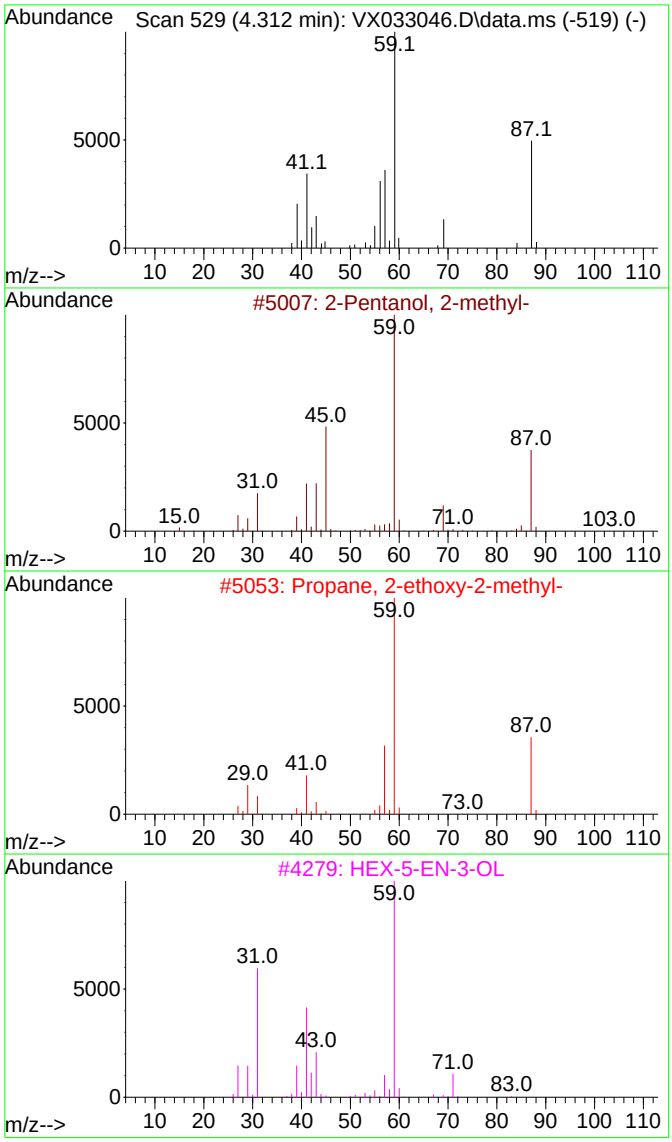
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

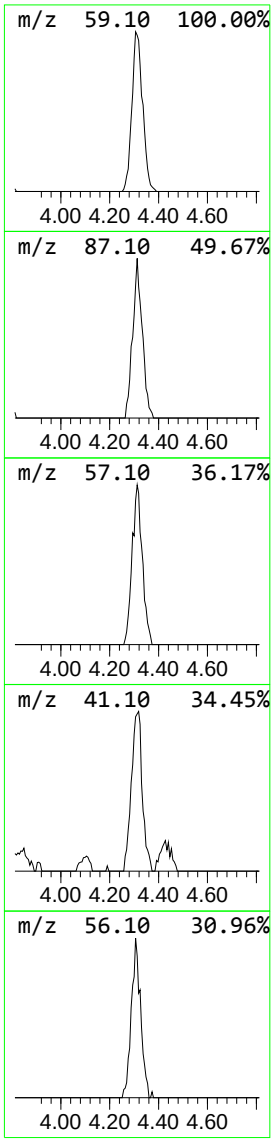
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.312	5.83 ug/l	44866	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	64
2	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	50
3	HEX-5-EN-3-OL	100	C6H12O	000688-99-3	47
4	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	38
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	28





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Instrument :
MSVOA_X
ClientSampleId :
MW-40

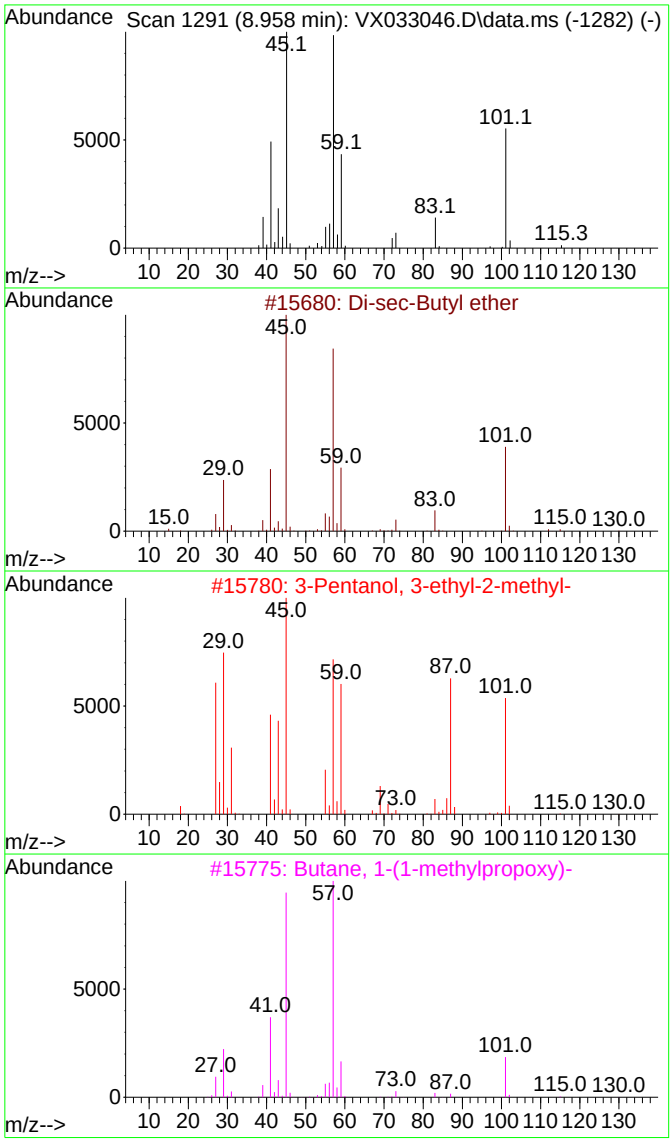
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

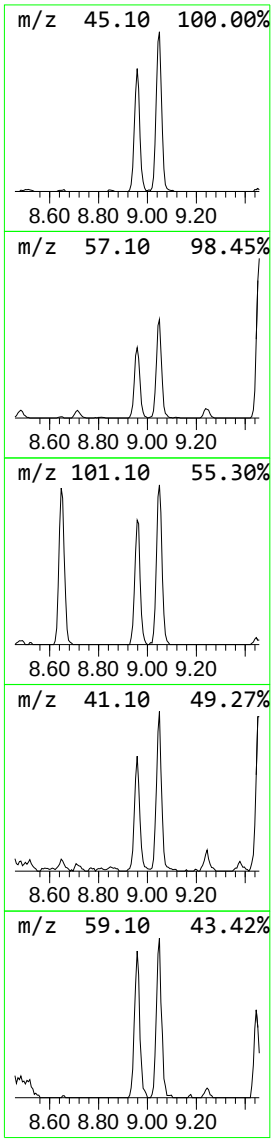
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Di-sec-Butyl ether Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.958	5.36 ug/l	63204	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	90
2	3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	64
3	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50
4	2-Hydroxy-3-pentanone	102	C5H10O2	005704-20-1	33
5	Boronic acid, ethyl-, diethyl ester	130	C6H15BO2	053907-92-9	33





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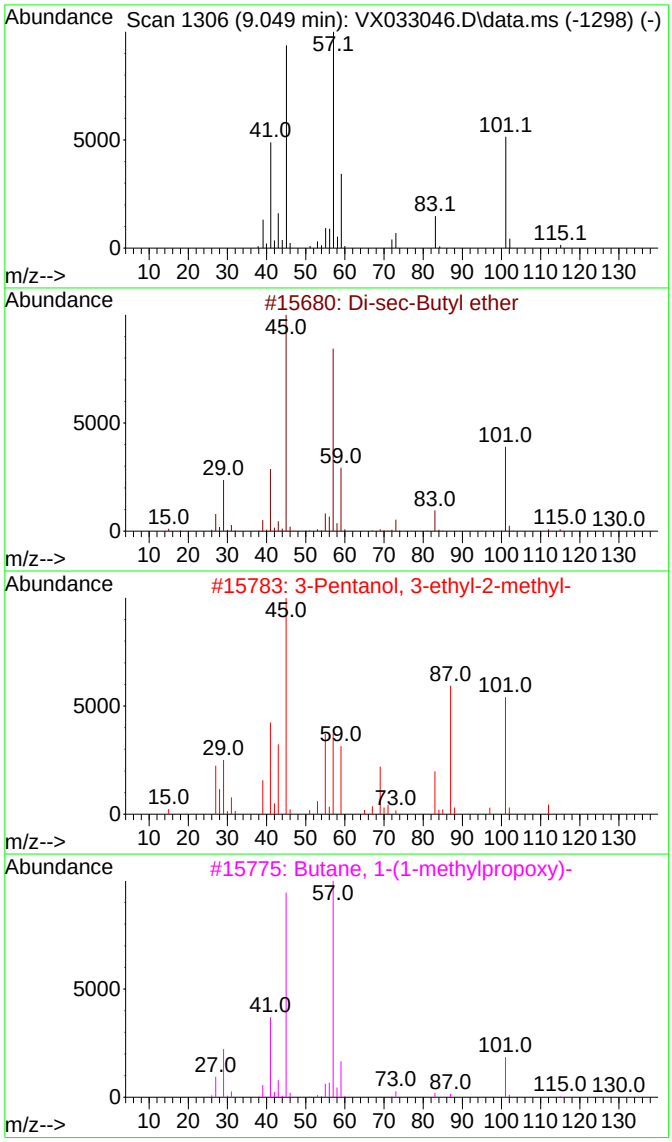
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

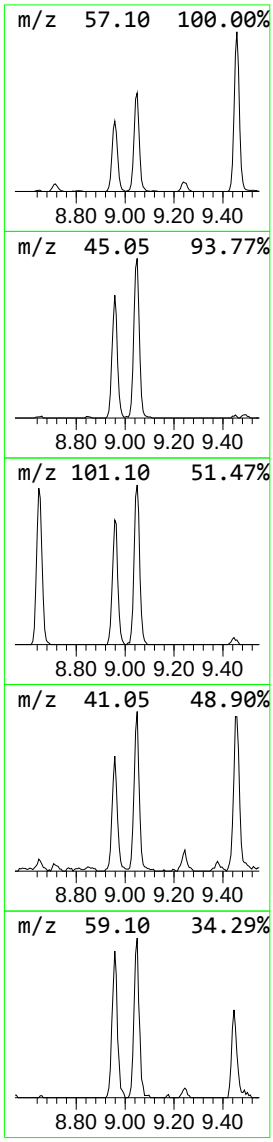
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 3-Pentanol, 3-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.049	6.60 ug/l	77839	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-sec-Butyl ether	130	C8H18O	006863-58-7	83
2	3-Pentanol, 3-ethyl-2-methyl-	130	C8H18O	000597-05-7	64
3	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
4	Fructofuranose, 2,6-anhydro-1,3,...	204	C9H16O5	004451-11-0	36
5	1-Octene, 3-(methoxymethoxy)-	172	C10H20O2	088738-34-5	33





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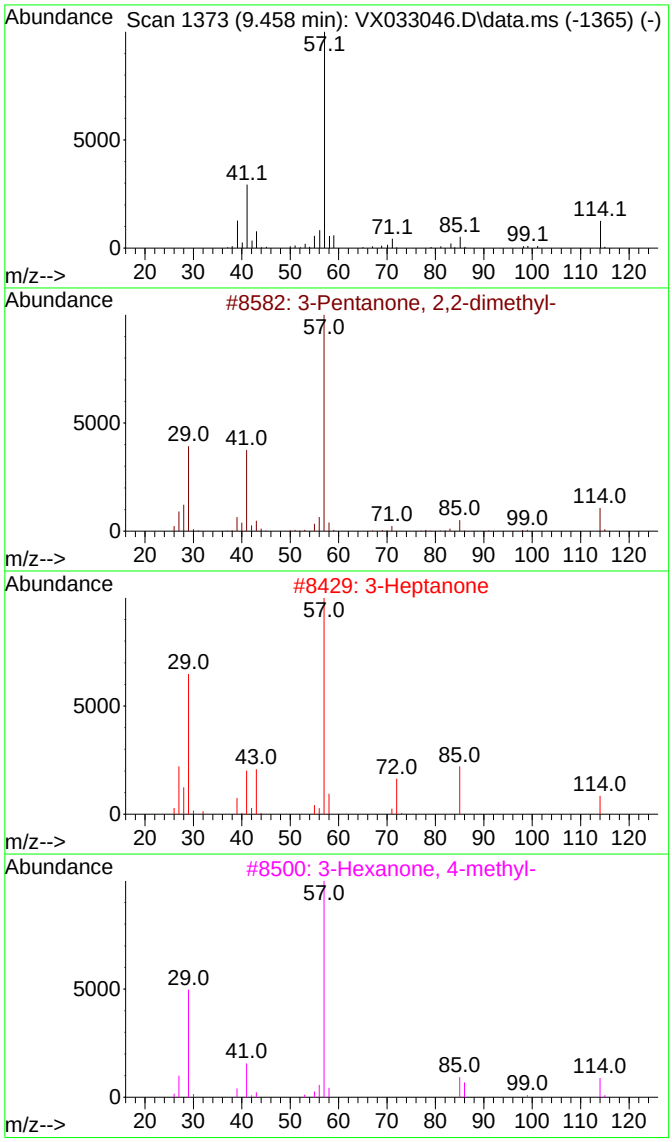
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

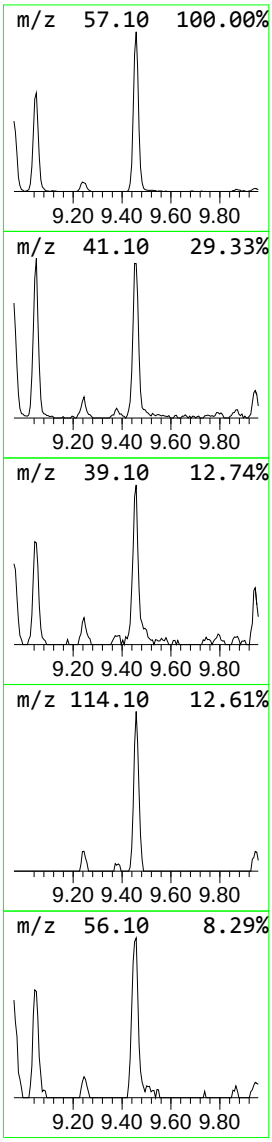
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 3-Pentanone, 2,2-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.458	6.29 ug/l	74188	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,2-dimethyl-	114	C7H14O	000564-04-5	80
2	3-Heptanone	114	C7H14O	000106-35-4	53
3	3-Hexanone, 4-methyl-	114	C7H14O	017042-16-9	53
4	2,2,5,5-Tetramethyl-3-hexanone	156	C10H20O	000868-91-7	50
5	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	47





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.246	57.0	ug/l	438454	1	5.556	384589	50.0
2-Pentanol, 2-m...	4.312	5.8	ug/l	44866	1	5.556	384589	50.0
Di-sec-Butyl ether	8.958	5.4	ug/l	63204	3	10.055	589301	50.0
3-Pentanol, 3-e...	9.049	6.6	ug/l	77839	3	10.055	589301	50.0
3-Pentanone, 2,...	9.458	6.3	ug/l	74188	3	10.055	589301	50.0