LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112922\
Data File : VX033115.D
Acq On : 29 Nov 2022 14:10
Operator : JC/MD
Sample : N5741-20
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 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: VX033115.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	42	rBV	220531	330224	21.83%	5.529%
2	2.989	301	312	325	rVV2	53245	202319	13.38%	3.387%
3	3.111	325	332	344	rVB	51724	120291	7.95%	2.014%
4	3.758	428	438	448	rBV	26457	71739	4.74%	1.201%
5	4.306	517	528	539	rBV2	14780	45274	2.99%	0.758%
6	5.385	691	705	717	rBV	62612	189078	12.50%	3.166%
7	5.550	723	732	750	rVB	135024	383844	25.38%	6.427%
8	5.958	789	799	804	rBV	67722	178473	11.80%	2.988%
9	6.038	804	812	828	rVB	571217	1512542	100.00%	25.324%
10	6.251	841	847	857	rVB4	6370	17638	1.17%	0.295%
11	6.763	919	931	944	rBV	204448	486499	32.16%	8.145%
12	8.427	1199	1204	1210	rBV2	22127	37949	2.51%	0.635%
13	8.647	1234	1240	1248	rBV	316159	497477	32.89%	8.329%
14	8.958	1282	1291	1300	rBV	38786	64765	4.28%	1.084%
15	9.049	1300	1306	1311	rBV	51063	78760	5.21%	1.319%
16	9.458	1364	1373	1385	rBV2	42522	76821	5.08%	1.286%
17	9.945	1448	1453	1459	rBV	15527	22429	1.48%	0.376%
18	10.055	1465	1471	1485	rVB	423957	579042	38.28%	9.695%
19	10.195	1490	1494	1501	rBV2	9070	15208	1.01%	0.255%
20	10.640	1563	1567	1573	rVB	13722	17702	1.17%	0.296%
21	10.964	1613	1620	1625	rBV	12496	17513	1.16%	0.293%
22	11.079	1634	1639	1649	rBV	274955	351802	23.26%	5.890%
23	11.616	1723	1727	1730	rBV	14670	18601	1.23%	0.311%
24	11.750	1745	1749	1755	rVB	13542	17339	1.15%	0.290%
25	12.024	1788	1794	1800	rBV	404572	534482	35.34%	8.949%
26	12.085	1800	1804	1812	rVB	16495	21969	1.45%	0.368%
27	12.244	1824	1830	1836	rBV	29309	38516	2.55%	0.645%
28	12.701	1900	1905	1911	rVB2	17705	25847	1.71%	0.433%
29	13.292	1998	2002	2007	rVB2	13822	18595	1.23%	0.311%

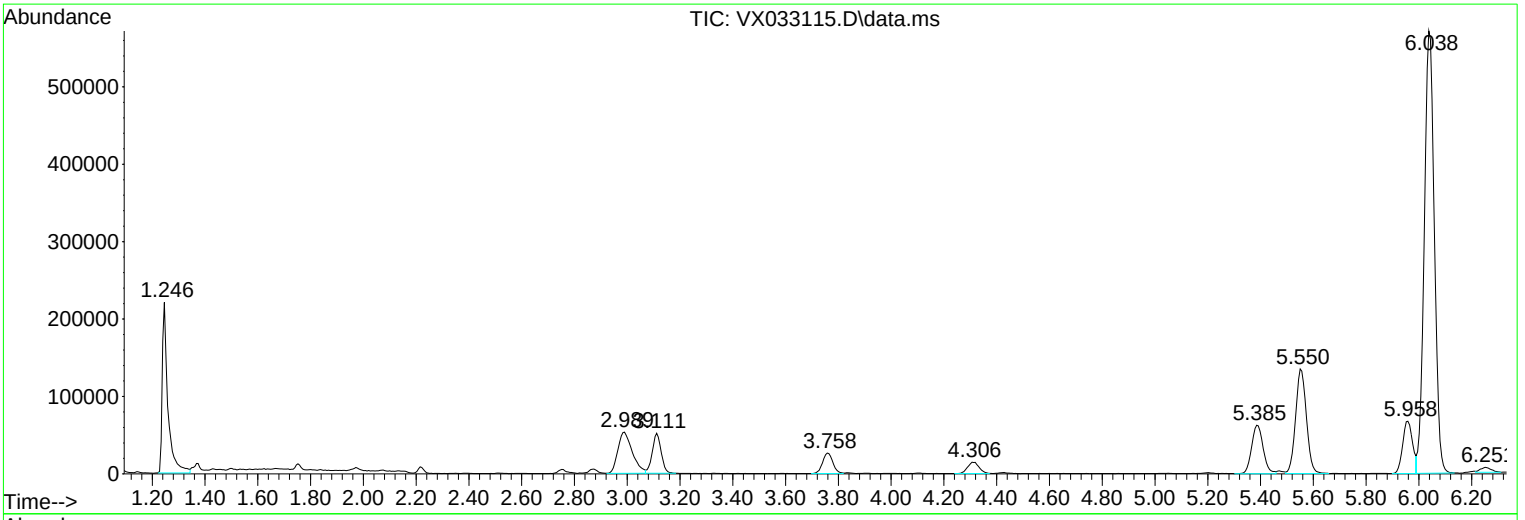
Sum of corrected areas: 5972738

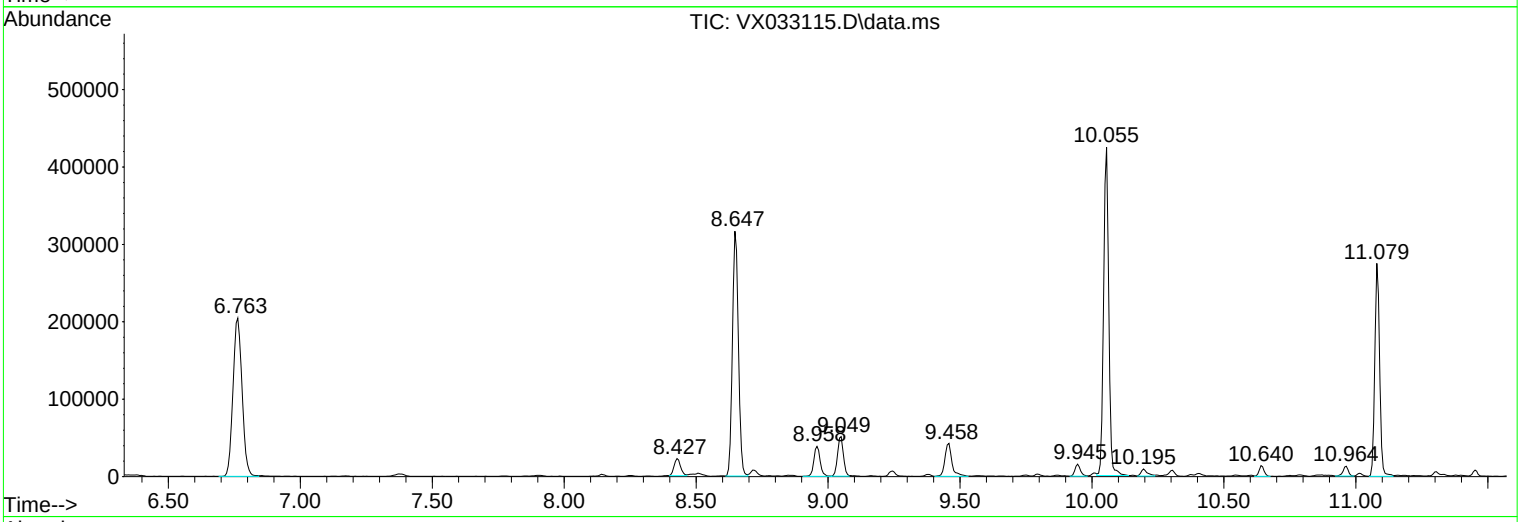
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112922\
Data File : VX033115.D
Acq On : 29 Nov 2022 14:10
Operator : JC/MD
Sample : N5741-20
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

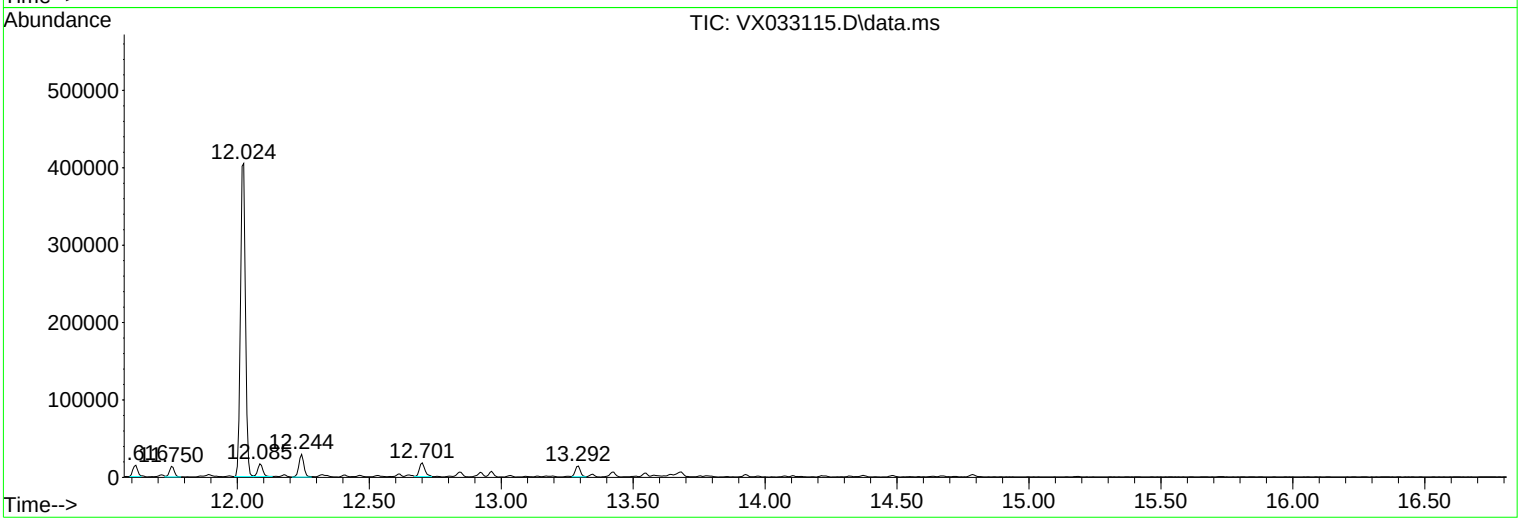
Instrument :
MSVOA_X
ClientSampleId :
MW-40

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112922\
Data File : VX033115.D
Acq On : 29 Nov 2022 14:10
Operator : JC/MD
Sample : N5741-20
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-40

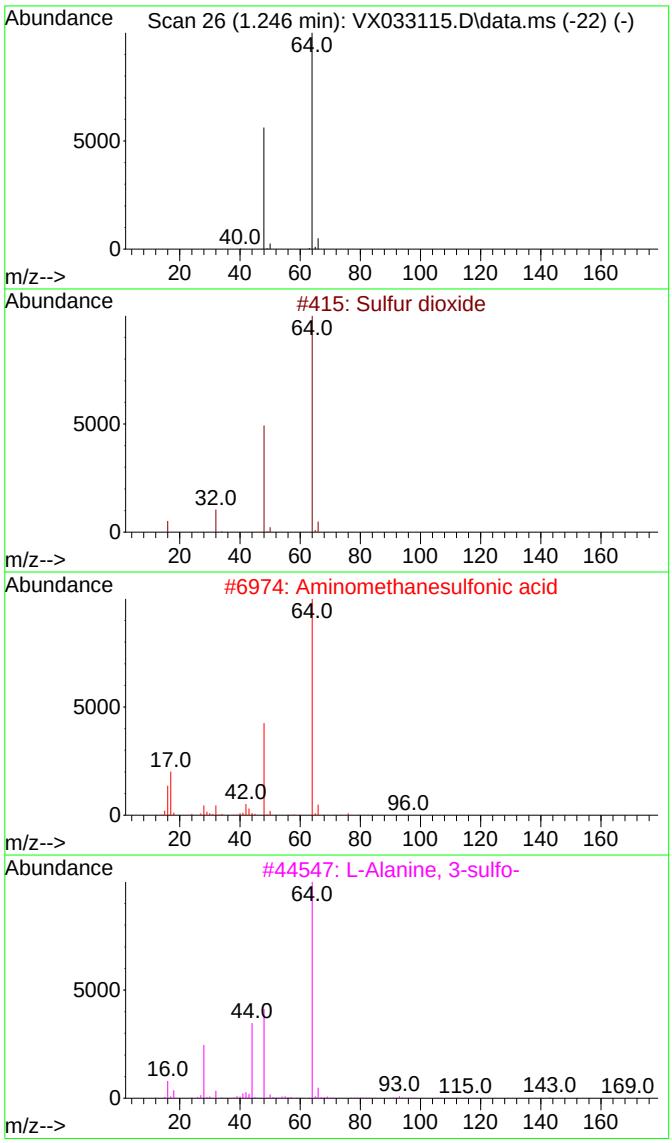
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

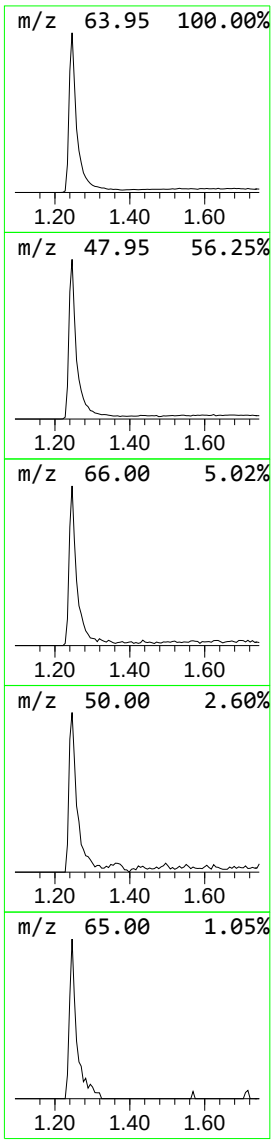
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	43.02 ug/l	330224	Pentafluorobenzene	5.550

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	Ethyl Chloride	64	C2H5Cl	000075-00-3	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112922\
Data File : VX033115.D
Acq On : 29 Nov 2022 14:10
Operator : JC/MD
Sample : N5741-20
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-40

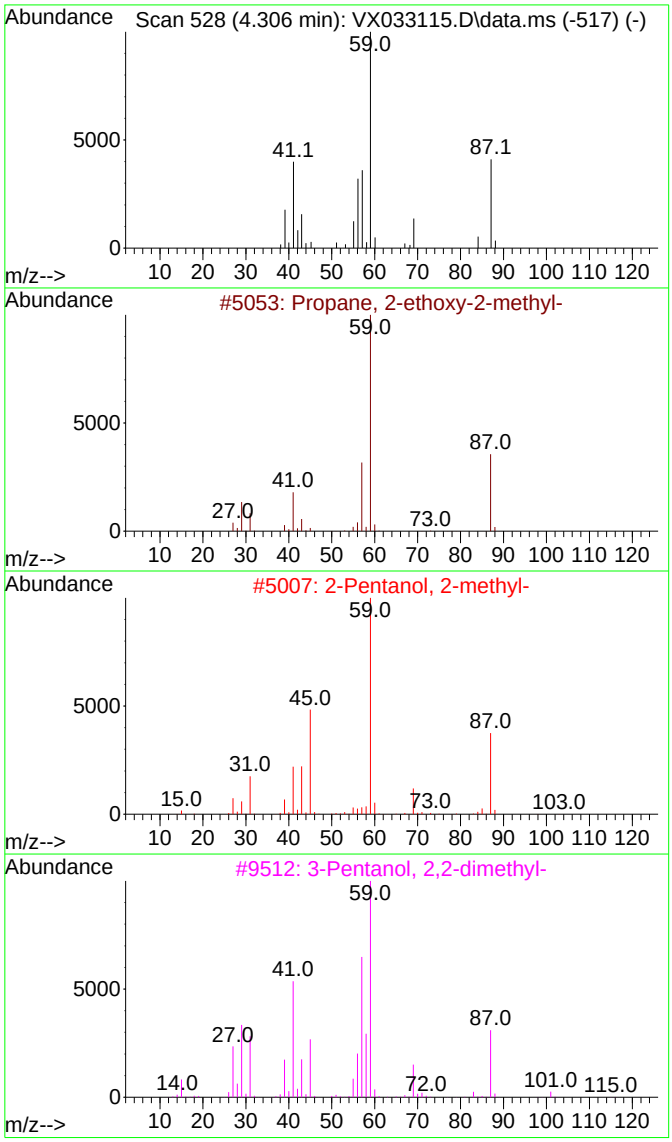
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

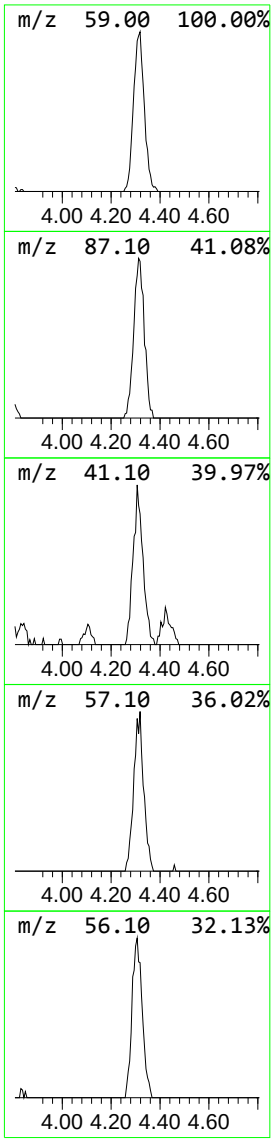
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Propane, 2-ethoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	5.90 ug/l	45274	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	64
2	2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	50
3	3-Pentanol, 2,2-dimethyl-	116	C7H16O	003970-62-5	39
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	38
5	HEX-5-EN-3-OL	100	C6H12O	000688-99-3	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112922\
Data File : VX033115.D
Acq On : 29 Nov 2022 14:10
Operator : JC/MD
Sample : N5741-20
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-40

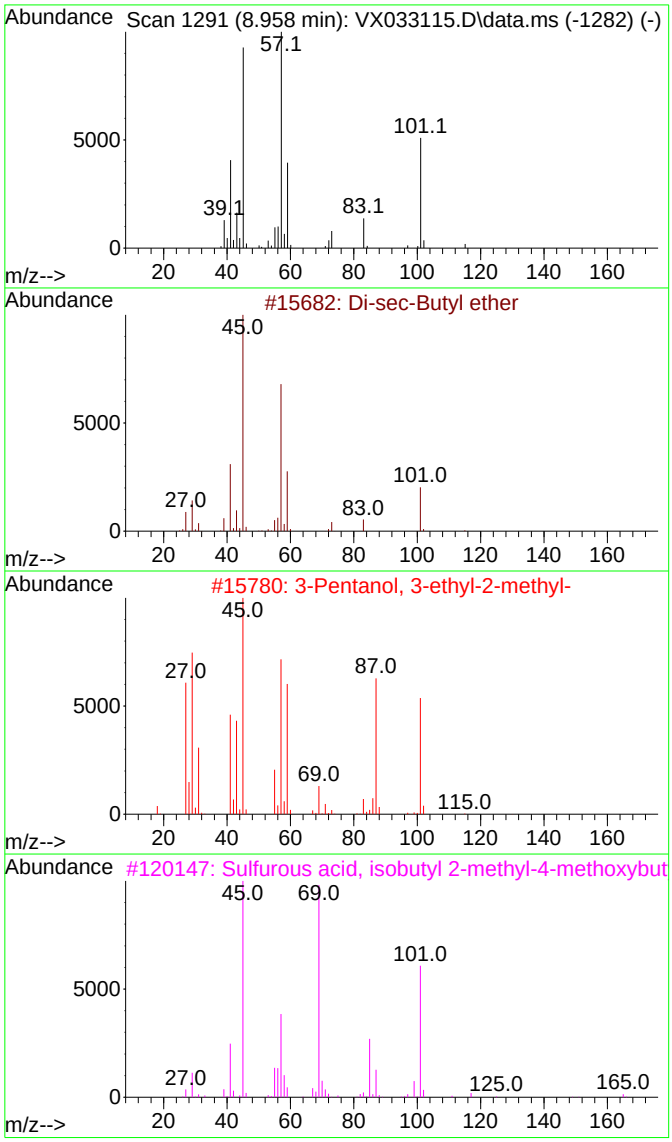
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

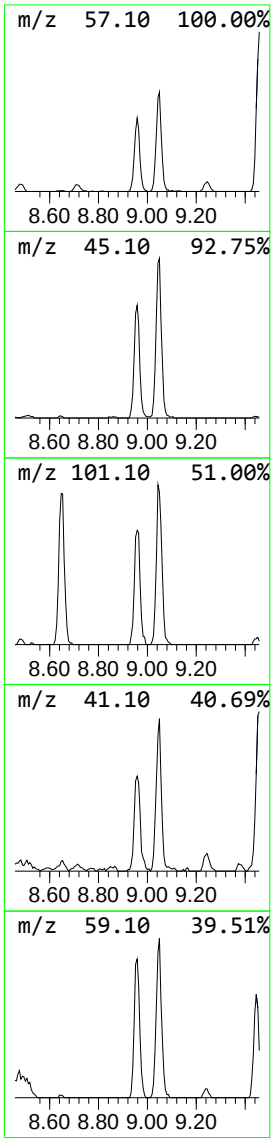
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.958	5.59 ug/l	64765	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	Sulfurous acid, isobutyl 2-methy...	238	C10H22O4S	1000309-20-3	50
4	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50
5	Butanoic acid, 4-methoxy-, methy...	132	C6H12O3	029006-01-7	45





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112922\
Data File : VX033115.D
Acq On : 29 Nov 2022 14:10
Operator : JC/MD
Sample : N5741-20
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-40

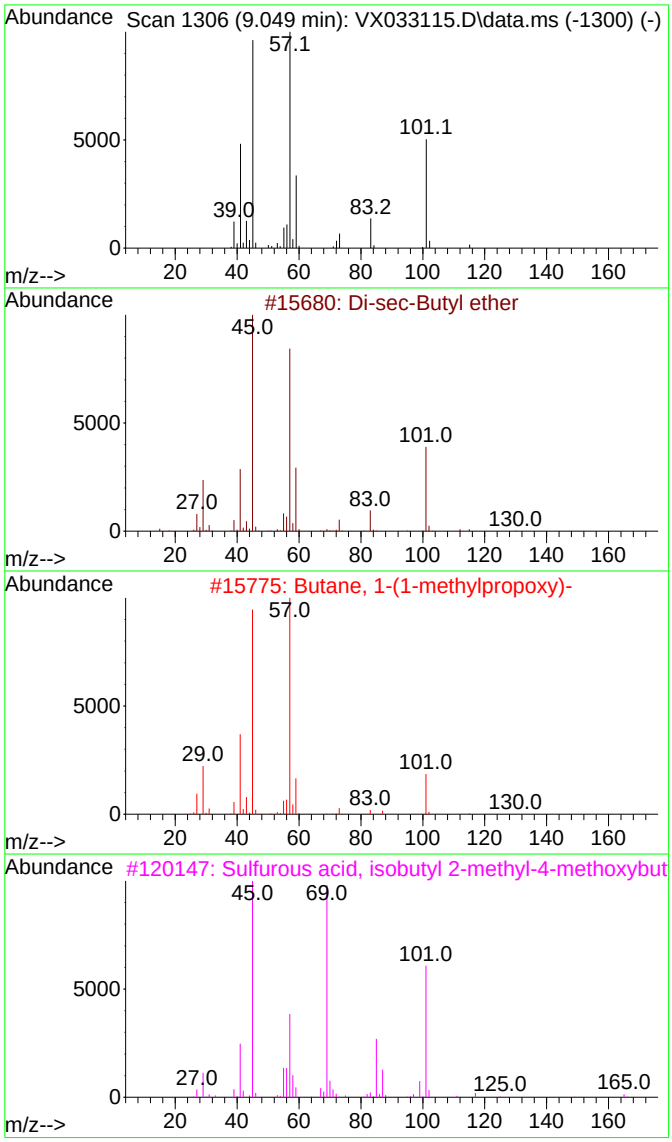
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

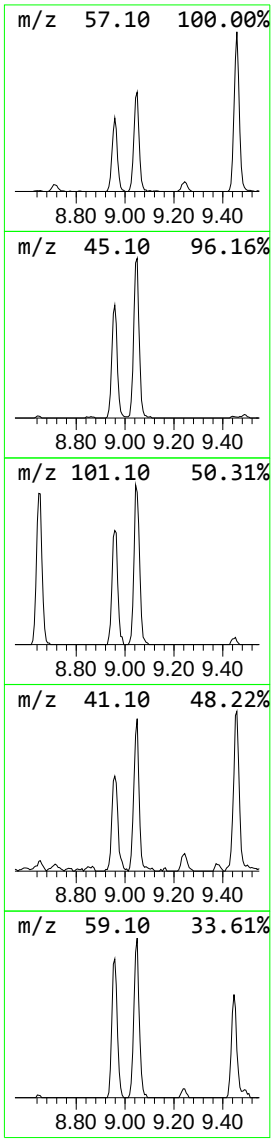
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butane, 1-(1-methylpropoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.049	6.80 ug/l	78760	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	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
3	Sulfurous acid, isobutyl 2-methy...	238	C10H22O4S	1000309-20-3	45
4	1-Octene, 3-(methoxymethoxy)-	172	C10H20O2	088738-34-5	40
5	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112922\
Data File : VX033115.D
Acq On : 29 Nov 2022 14:10
Operator : JC/MD
Sample : N5741-20
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-40

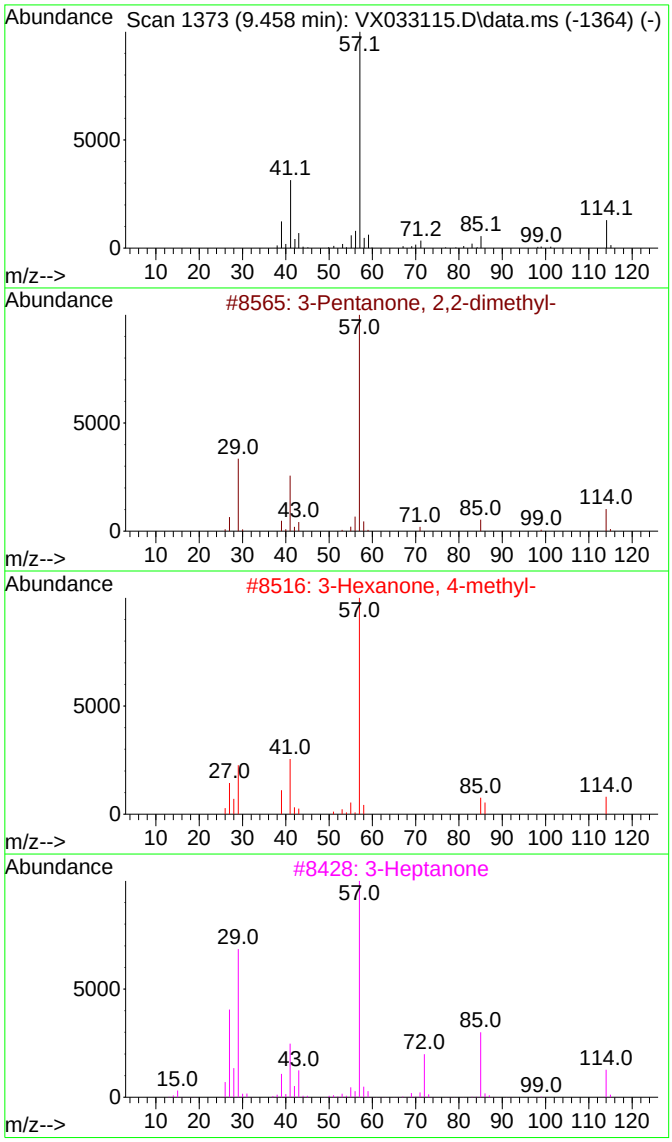
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X112222W.M
Quant Title : SW846 8260

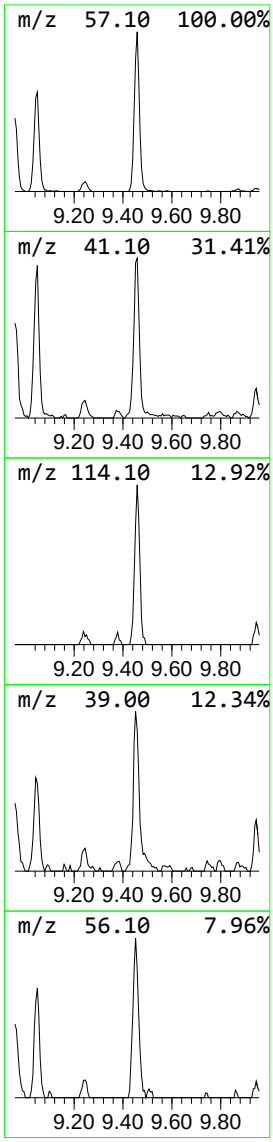
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.458	6.63 ug/l	76821	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-Hexanone, 4-methyl-	114	C7H14O	017042-16-9	64
3	3-Heptanone	114	C7H14O	000106-35-4	59
4	2,2,5,5-Tetramethyl-3-hexanone	156	C10H20O	000868-91-7	50
5	3-Hexanone, 5-methyl-	114	C7H14O	000623-56-3	50





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX112922\
Data File : VX033115.D
Acq On : 29 Nov 2022 14:10
Operator : JC/MD
Sample : N5741-20
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.246	43.0	ug/l	330224	1	5.550	383844	50.0
Propane, 2-etho...	4.306	5.9	ug/l	45274	1	5.550	383844	50.0
Di-sec-Butyl ether	8.958	5.6	ug/l	64765	3	10.055	579042	50.0
Butane, 1-(1-me...	9.049	6.8	ug/l	78760	3	10.055	579042	50.0
3-Pentanone, 2,...	9.458	6.6	ug/l	76821	3	10.055	579042	50.0