LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN120823\
Data File : VN080411.D
Acq On : 08 Dec 2023 17:09
Operator : JC\MD
Sample : 05729-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
STORAGE-BLANK-WATER-REF-5

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_N\methods\82N111623W.M
Title : SW846 8260

Signal : TIC: VN080411.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.301	52	59	67	rBV	80341	210036	10.36%	1.389%
2	2.665	119	121	126	rVB3	24259	31742	1.57%	0.210%
3	8.165	1048	1056	1061	rBV	272831	657986	32.46%	4.350%
4	8.224	1061	1066	1077	rVB	406948	903177	44.56%	5.971%
5	8.582	1119	1127	1137	rBV	267478	595857	29.40%	3.939%
6	9.100	1206	1215	1224	rBV	633034	1300556	64.17%	8.598%
7	10.571	1457	1465	1474	rBV	1009665	1887720	93.14%	12.479%
8	11.865	1677	1685	1694	rVB	948657	1711150	84.43%	11.312%
9	12.076	1714	1721	1724	rBV7	11796	22627	1.12%	0.150%
10	12.853	1845	1853	1860	rBV	817131	1414110	69.77%	9.348%
11	12.953	1865	1870	1876	rBV2	116515	202005	9.97%	1.335%
12	13.176	1901	1908	1914	rBV4	29477	47901	2.36%	0.317%
13	13.794	2006	2013	2020	rVB	926196	1570692	77.50%	10.384%
14	14.329	2096	2104	2106	rBV6	15871	30886	1.52%	0.204%
15	15.711	2331	2339	2341	rBV	801552	1450302	71.56%	9.588%
16	15.741	2341	2344	2353	rVB	1170213	2026799	100.00%	13.399%
17	15.988	2378	2386	2397	rVB	425831	878370	43.34%	5.807%
18	16.541	2469	2480	2481	rBV7	92010	184724	9.11%	1.221%

Sum of corrected areas: 15126640

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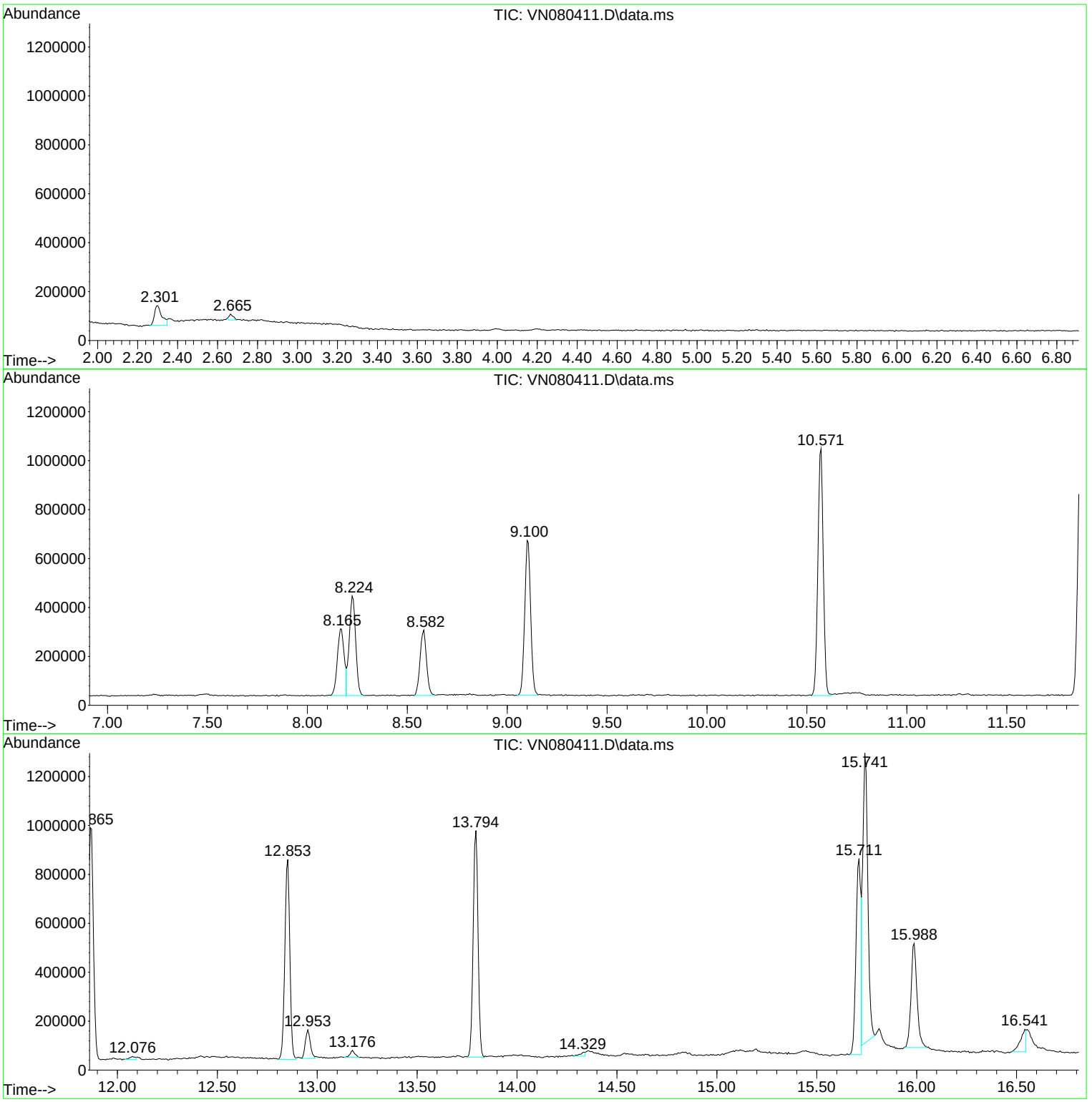
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
STORAGE-BLANK-WATER-REF-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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



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Data File : VN080411.D
Acq On : 08 Dec 2023 17:09
Operator : JC\MD
Sample : 05729-02
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
STORAGE-BLANK-WATER-REF-5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

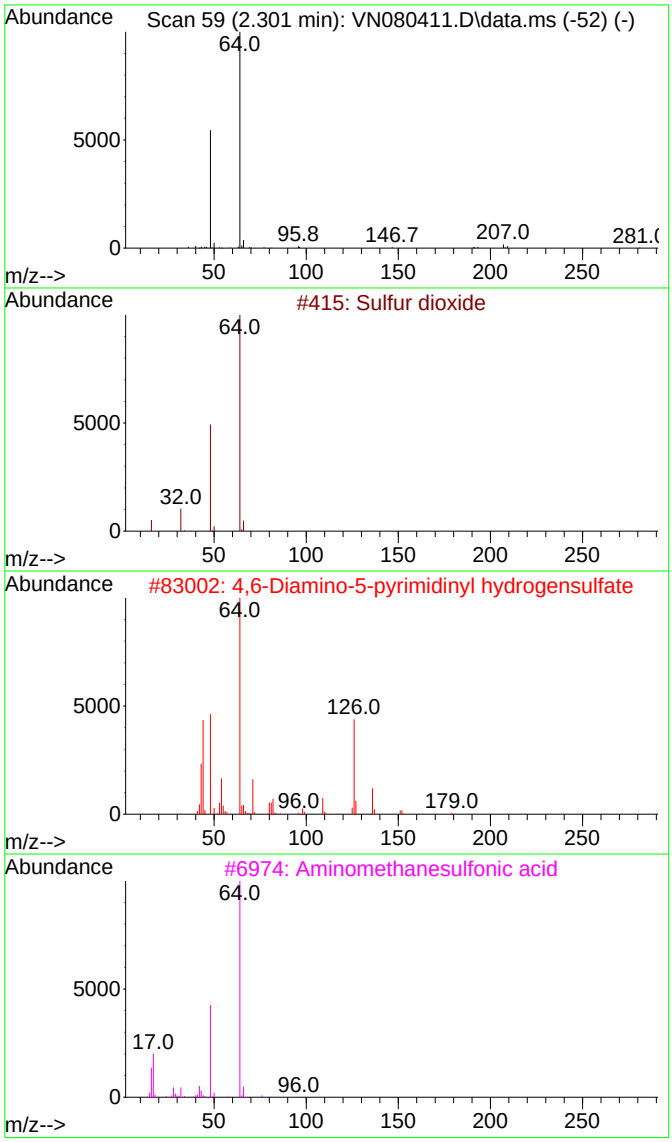
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

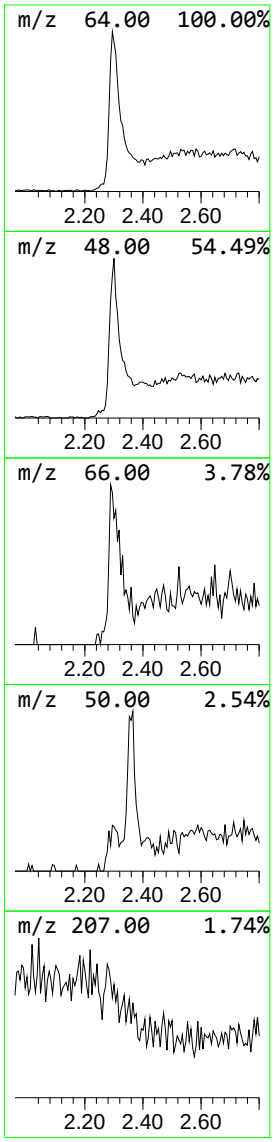
****

Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.301	11.63 ug/l	210036	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	4,6-Diamino-5-pyrimidinyl hydrog...	206	C4H6N4O4S	071525-41-2	9
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4	Thiosulfuric acid (H2S2O3), S-(2...	320	C11H16N2O3S3	040284-00-2	9
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4





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Acq On : 08 Dec 2023 17:09
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
STORAGE-BLANK-WATER-REF-5

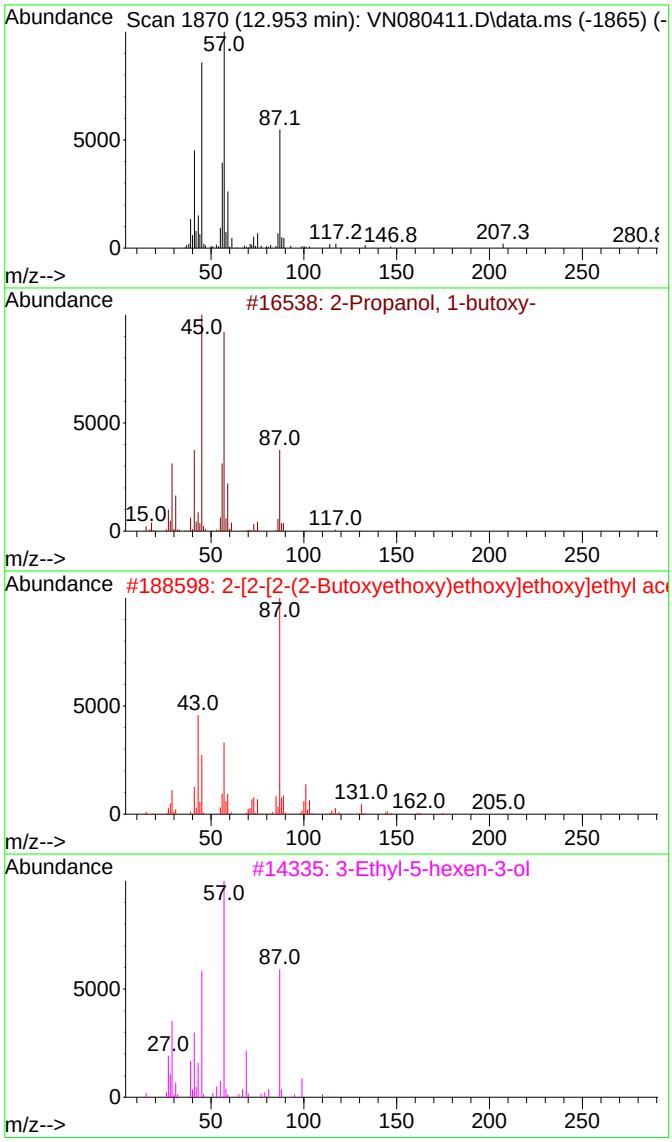
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

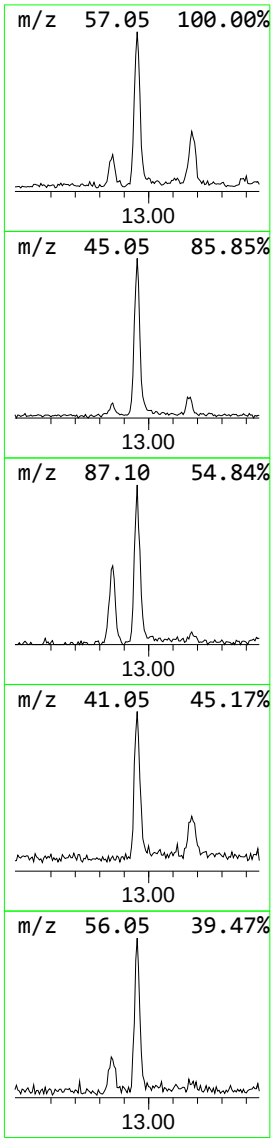
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Propanol, 1-butoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.953	6.43 ug/l	202005	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	78
2	2-[2-[2-(2-Butoxyethoxy)ethoxy]e...	292	C14H28O6	1000351-93-9	56
3	3-Ethyl-5-hexen-3-ol	128	C8H16O	001907-46-6	50
4	2-Ethyl-2-hydroxybutyric acid	132	C6H12O3	003639-21-2	50
5	Propane, 1,1'-[ethylidenebis(oxy...	146	C8H18O2	000105-82-8	47





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Operator : JC\MD
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
STORAGE-BLANK-WATER-REF-5

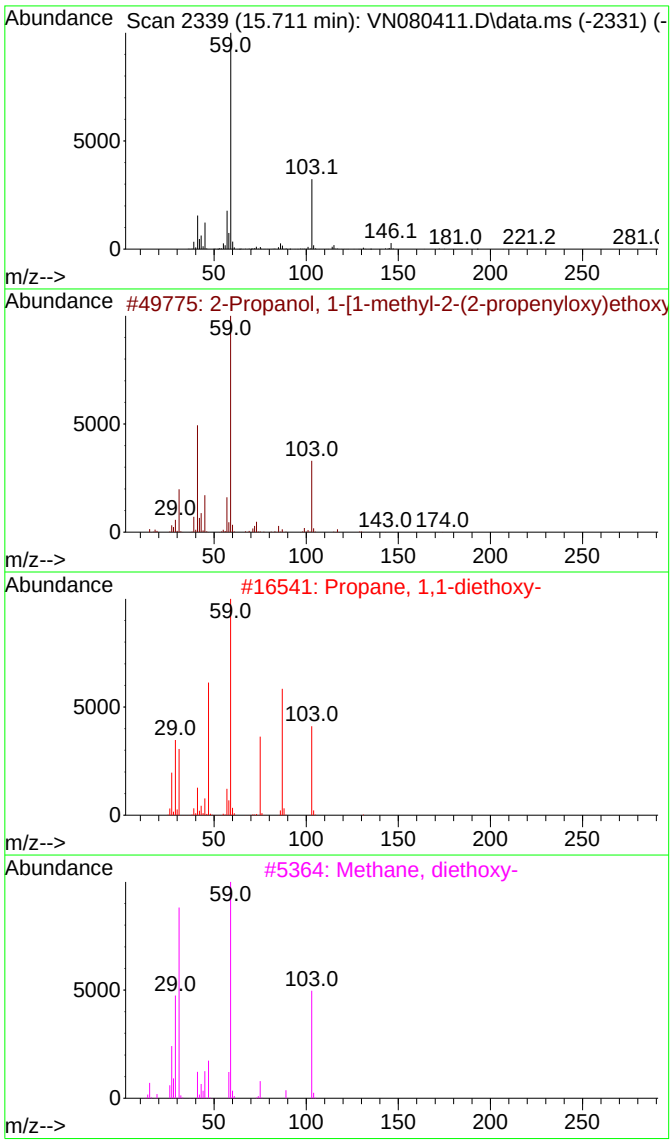
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

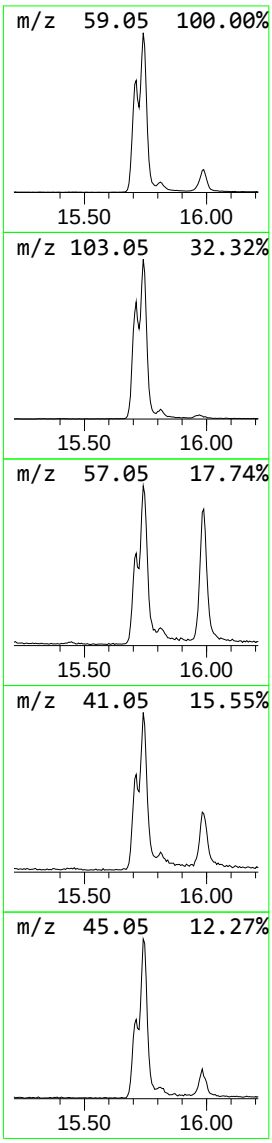
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanol, 1-[1-methyl-2-(... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.711	46.17 ug/l	1450300	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	83
2	Propane, 1,1-diethoxy-	132	C7H16O2	004744-08-5	78
3	Methane, diethoxy-	104	C5H12O2	000462-95-3	72
4	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	72
5	1-(1-tert-Butoxypropan-2-yloxy)p...	190	C10H22O3	132739-31-2	72





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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
STORAGE-BLANK-WATER-REF-5

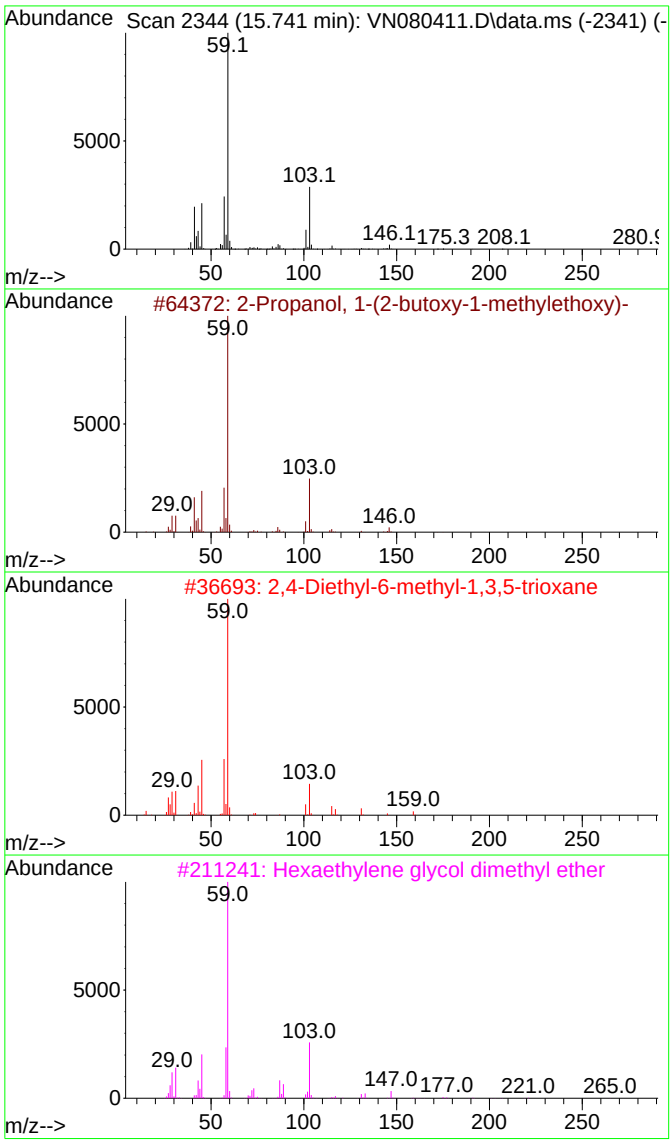
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

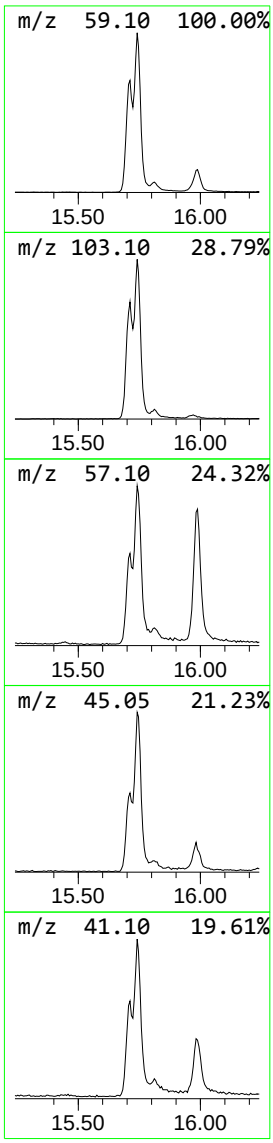
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.741	64.52 ug/l	2026800	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	90
2	2,4-Diethyl-6-methyl-1,3,5-trioxane	160	C8H16O3	117888-04-7	78
3	Hexaethylene glycol dimethyl ether	310	C14H30O7	001072-40-8	78
4	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	72
5	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	64





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
STORAGE-BLANK-WATER-REF-5

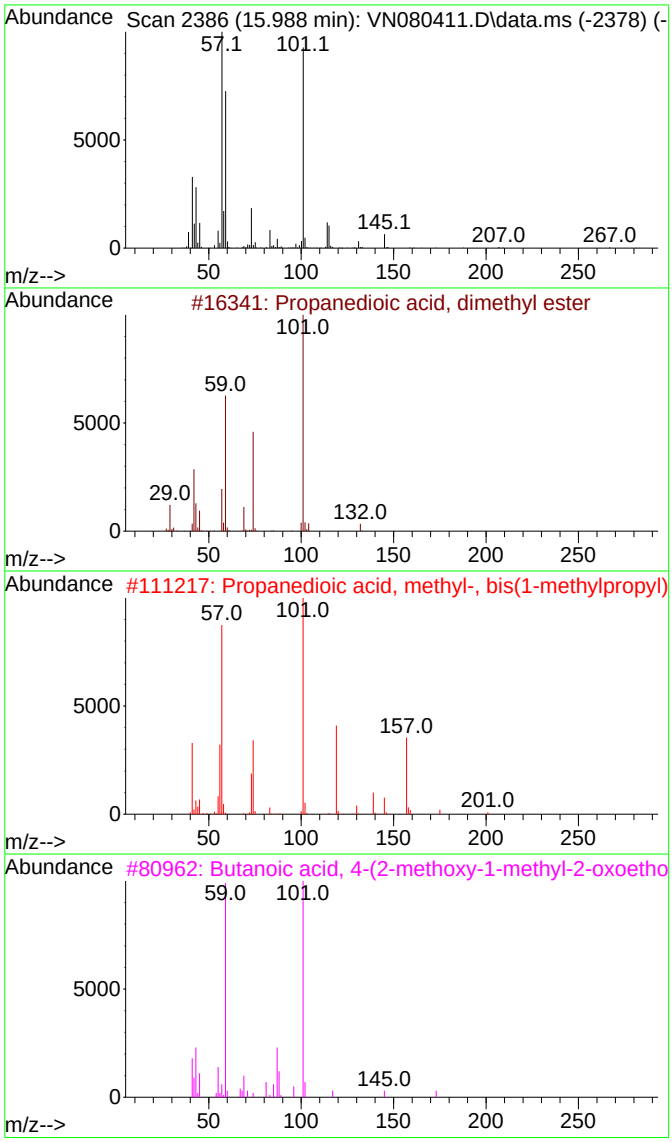
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

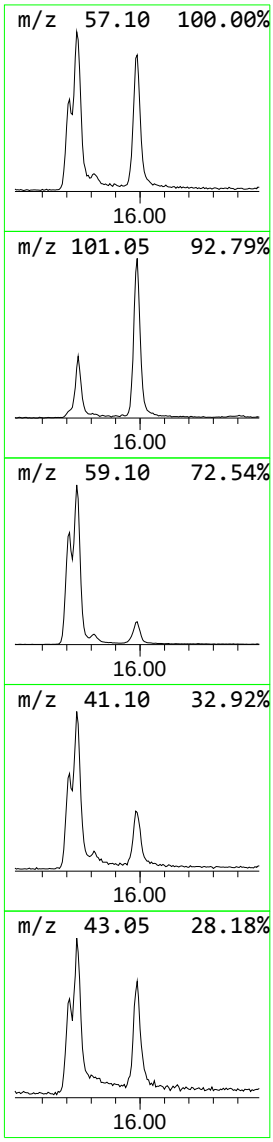
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Propanedioic acid, dimethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.988	27.96 ug/l	878370	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanedioic acid, dimethyl ester	132	C5H8O4	000108-59-8	53
2	Propanedioic acid, methyl-, bis(...	230	C12H22O4	057983-27-4	50
3	Butanoic acid, 4-(2-methoxy-1-me...	204	C9H16O5	054966-46-0	50
4	3-Hexanol, 3-ethyl-	130	C8H18O	000597-76-2	40
5	Butanedioic acid, monomethyl ester	132	C5H8O4	003878-55-5	40





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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
STORAGE-BLANK-WATER-REF-5

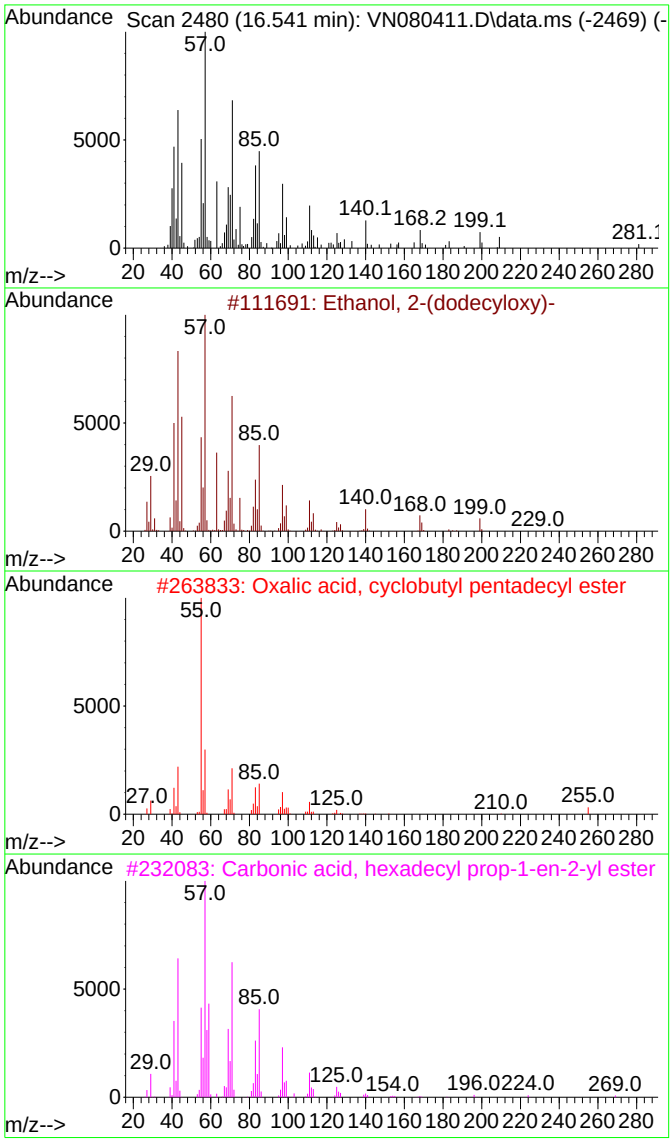
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

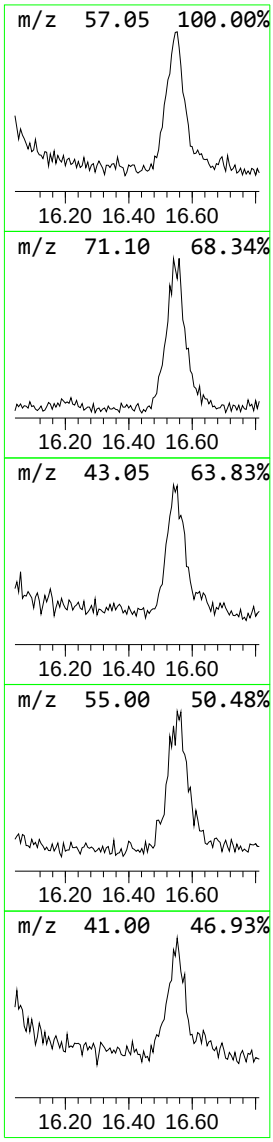
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Ethanol, 2-(dodecyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.541	5.88 ug/l	184724	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	72
2	Oxalic acid, cyclobutyl pentadec...	354	C21H38O4	1010309-70-5	62
3	Carbonic acid, hexadecyl prop-1-...	326	C20H38O3	1000382-90-3	58
4	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	58
5	Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	58





Tentatively Identified Compound (LSC) summary

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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	2.301	11.6	ug/l	210036	1	8.224	903177	50.0
2-Propanol, 1-b...	12.953	6.4	ug/l	202005	4	13.794	1570690	50.0
2-Propanol, 1-[...	15.711	46.2	ug/l	1450300	4	13.794	1570690	50.0
2-Propanol, 1-(...	15.741	64.5	ug/l	2026800	4	13.794	1570690	50.0
Propanedioic ac...	15.988	28.0	ug/l	878370	4	13.794	1570690	50.0
Ethanol, 2-(dod...	16.541	5.9	ug/l	184724	4	13.794	1570690	50.0