LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028765.D
Acq On : 17 May 2022 18:05
Operator : JC/MD
Sample : N2884-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31517

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\82X051222W.M
Title : SW846 8260

Signal : TIC: VX028765.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.447	55	59	72	rBV	9097843	13001905	11.56%	3.100%
2	2.288	189	197	206	rBV	17661283	70185934	62.42%	16.732%
3	2.392	212	214	217	rVB	13542190	12649527	11.25%	3.016%
4	2.428	217	220	237	rVB2	5833066	8965682	7.97%	2.137%
5	4.117	444	497	501	rBV	10963689	112434892	100.00%	26.803%
6	4.270	512	522	533	rBV	964666	2569011	2.28%	0.612%
7	5.562	723	734	748	rVB	444712	1263279	1.12%	0.301%
8	6.769	923	932	942	rVV	730124	1749049	1.56%	0.417%
9	6.885	942	951	964	rVB	836868	1998658	1.78%	0.476%
10	7.220	995	1006	1013	rBV3	614104	1604082	1.43%	0.382%
11	7.586	1060	1066	1073	rVB	1052176	1952512	1.74%	0.465%
12	8.653	1234	1241	1249	rBV	1498588	2414481	2.15%	0.576%
13	8.872	1271	1277	1291	rVB	1759807	2861569	2.55%	0.682%
14	9.025	1291	1302	1307	rBV	38886272	81425940	72.42%	19.411%
15	9.183	1319	1328	1333	rBV	31595895	56046783	49.85%	13.361%
16	9.488	1373	1378	1384	rBV	2417570	3108124	2.76%	0.741%
17	10.086	1464	1476	1483	rBV2	9776966	15276540	13.59%	3.642%
18	10.159	1483	1488	1498	rVV	2666977	3304809	2.94%	0.788%
19	10.714	1571	1579	1584	rBV	1635212	2676491	2.38%	0.638%
20	11.085	1635	1640	1645	rVB	1372687	1787940	1.59%	0.426%
21	11.153	1645	1651	1656	rBV	2845649	3789801	3.37%	0.903%
22	11.659	1731	1734	1746	rVB	1174141	1859380	1.65%	0.443%
23	11.957	1776	1783	1788	rBV	10502967	12634239	11.24%	3.012%
24	12.024	1790	1794	1798	rBV	1541924	1807574	1.61%	0.431%
25	12.219	1821	1826	1831	rBV	1760084	2110576	1.88%	0.503%

Sum of corrected areas: 419478778

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ClientSampleId :
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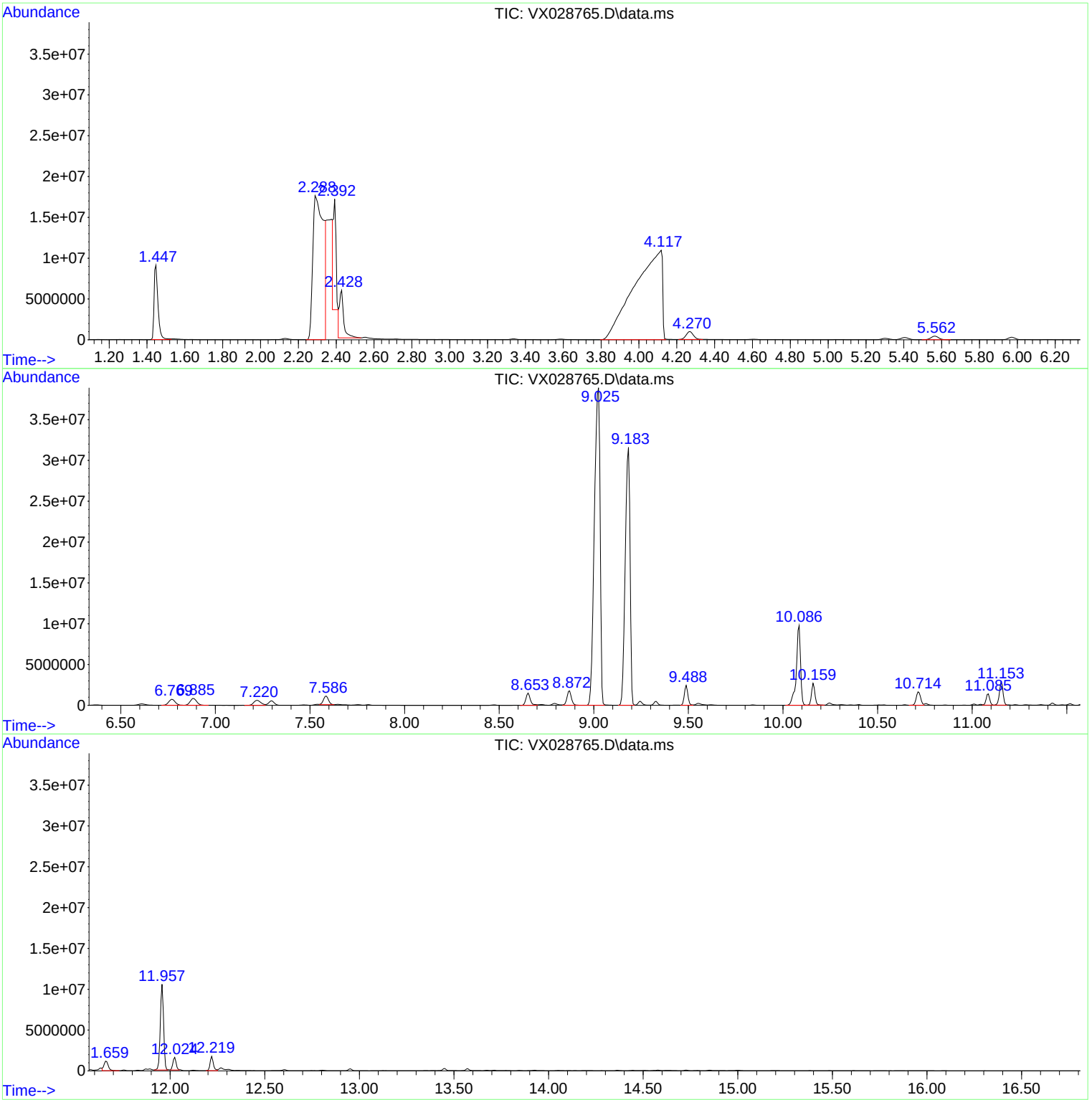
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

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



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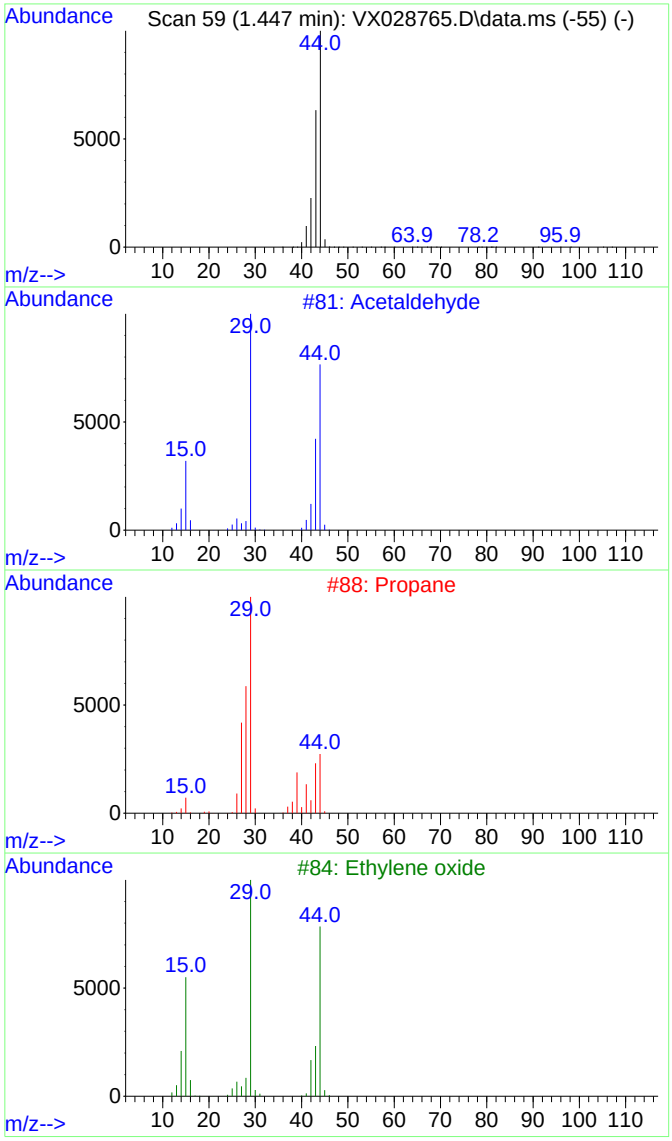
Quant Title : SW846 8260

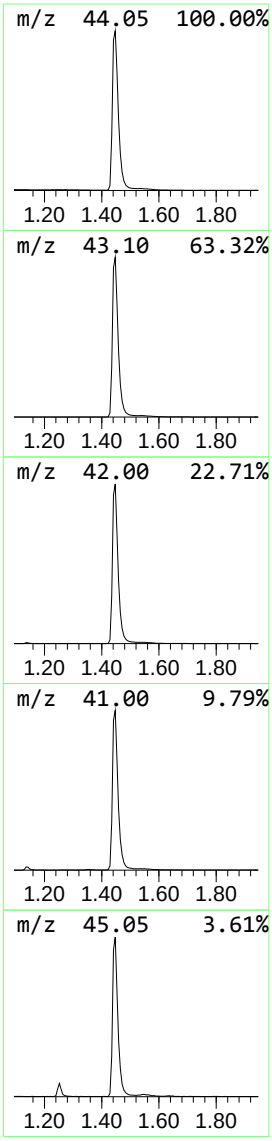
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.447	514.61 ug/l	13001900	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	64
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Alanine	89	C3H7NO2	000056-41-7	4
5	Hydrogen isocyanate	43	CHNO	000075-13-8	3





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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

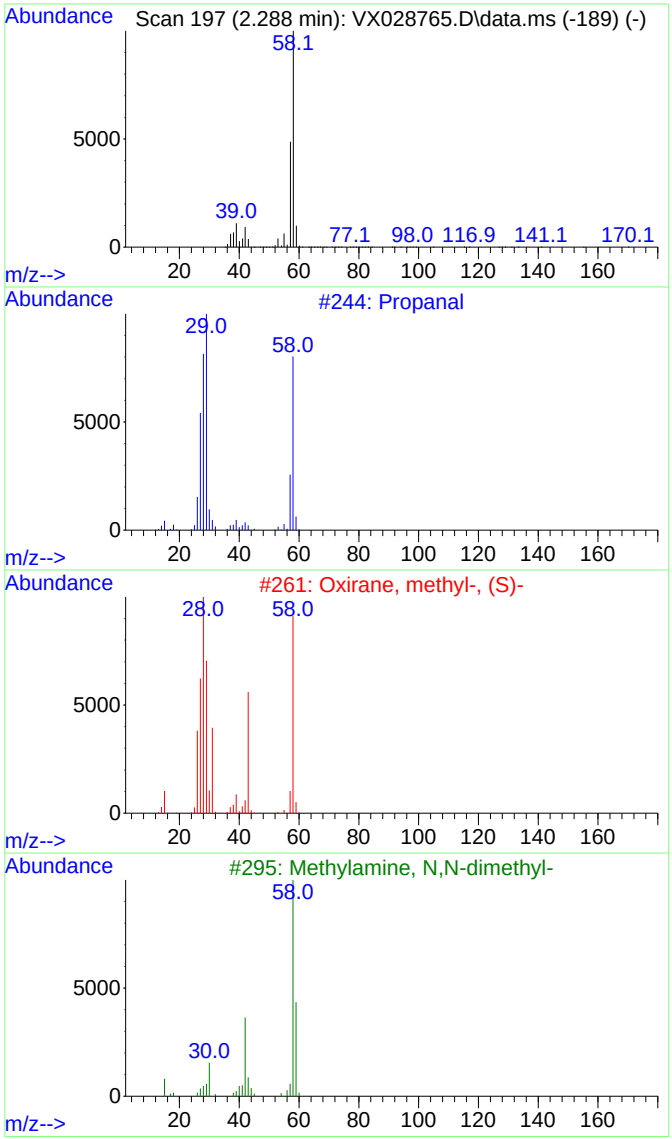
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

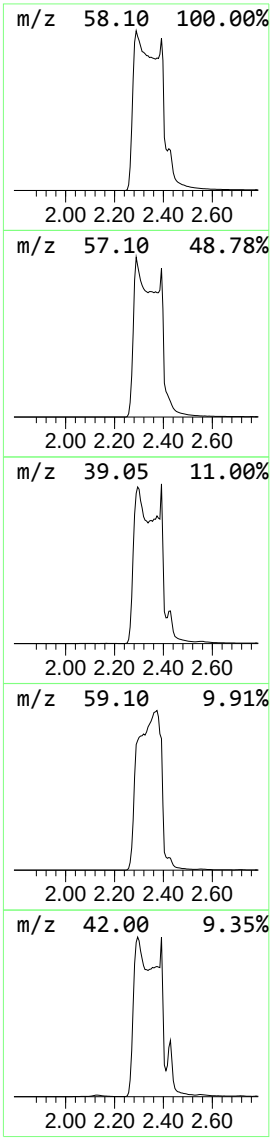
****

Peak Number 2 Propanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.288	2777.93 ug/l	70185900	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	56
2	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7
3	Methylamine, N,N-dimethyl-	59	C3H9N	000075-50-3	5
4	Propylene oxide	58	C3H6O	000075-56-9	4
5	2-Propen-1-amine	57	C3H7N	000107-11-9	4





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Operator : JC/MD
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31517

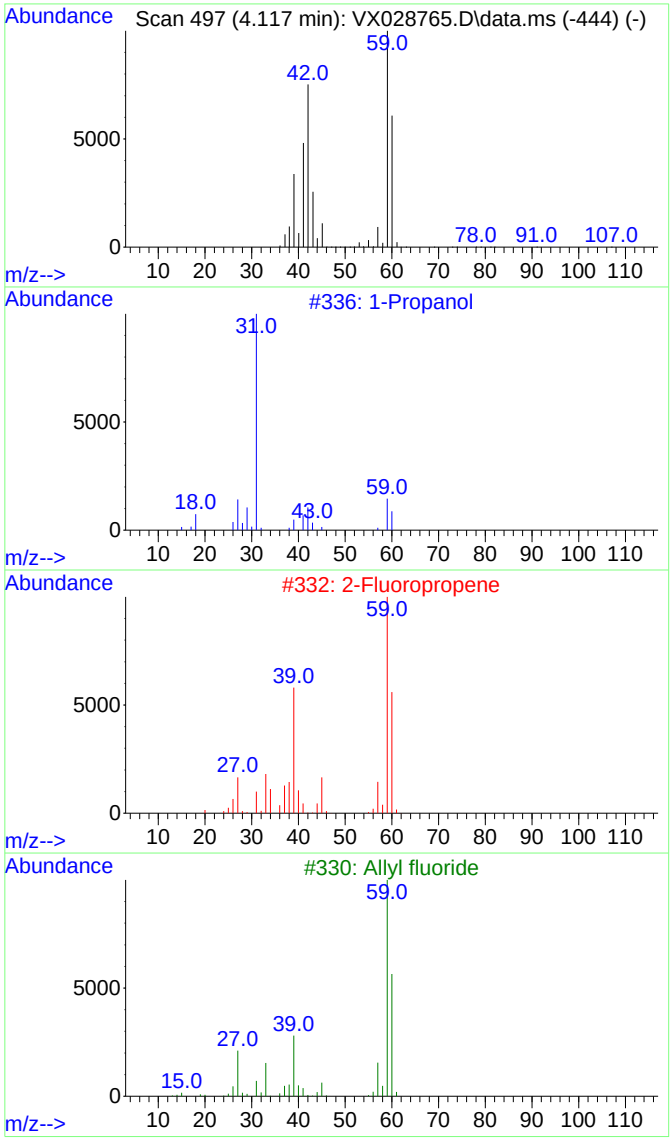
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

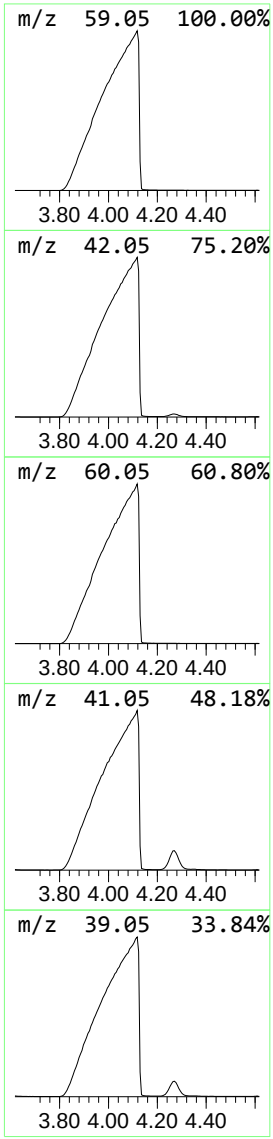
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.117	4450.12 ug/l	112435000	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	78
2	2-Fluoropropene	60	C3H5F	001184-60-7	43
3	Allyl fluoride	60	C3H5F	000818-92-8	38
4	Cyclopropane	42	C3H6	000075-19-4	16
5	Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	9





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Instrument :
MSVOA_X
ClientSampleId :
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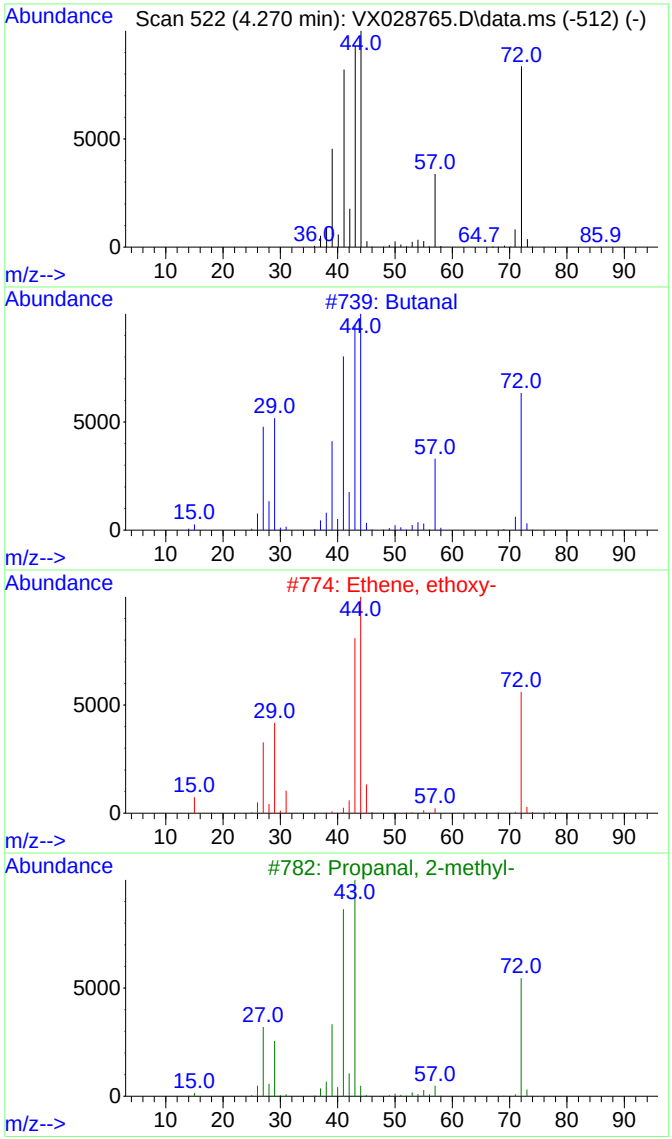
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

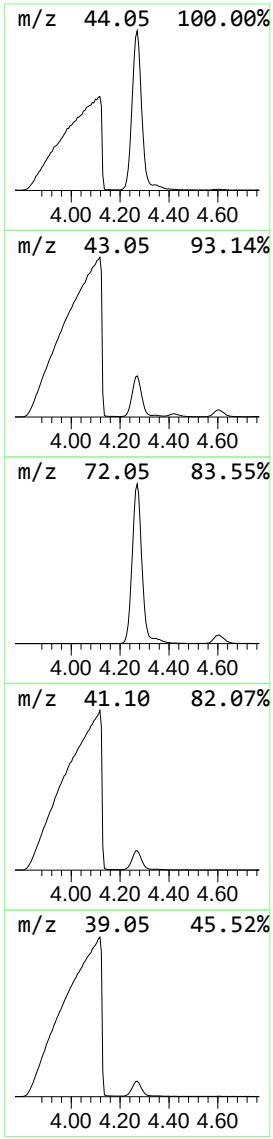
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.270	101.68 ug/l	2569010	Pentafluorobenzene	5.562

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	58
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	43
5	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	38





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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31517

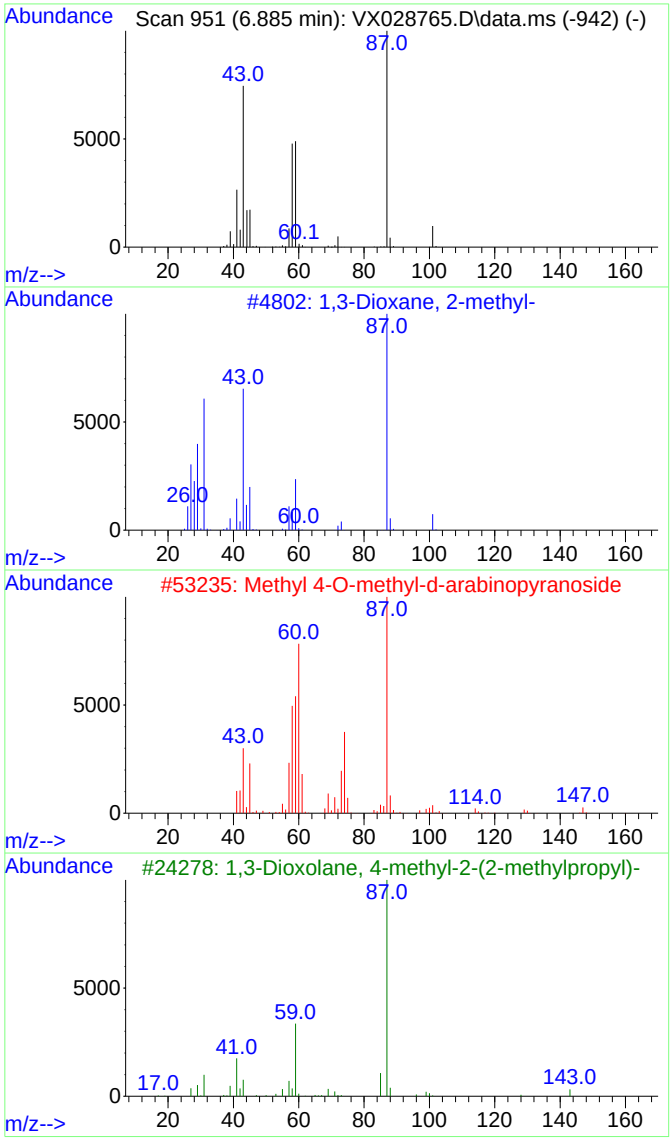
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

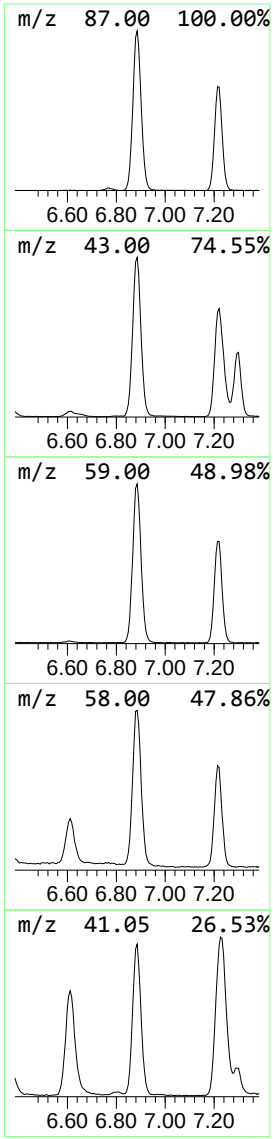
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,3-Dioxane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.885	57.14 ug/l	1998660	1,4-Difluorobenzene	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	52
2	Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	38
3	1,3-Dioxolane, 4-methyl-2-(2-met...	144	C8H16O2	018433-93-7	38
4	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	38
5	Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	37





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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31517

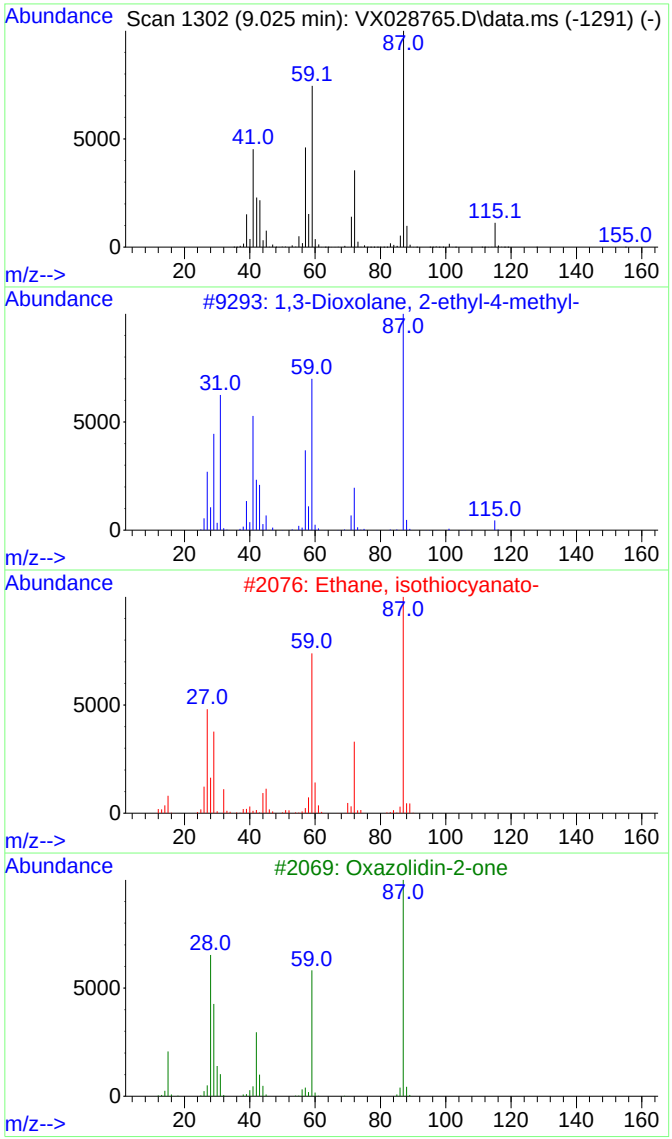
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

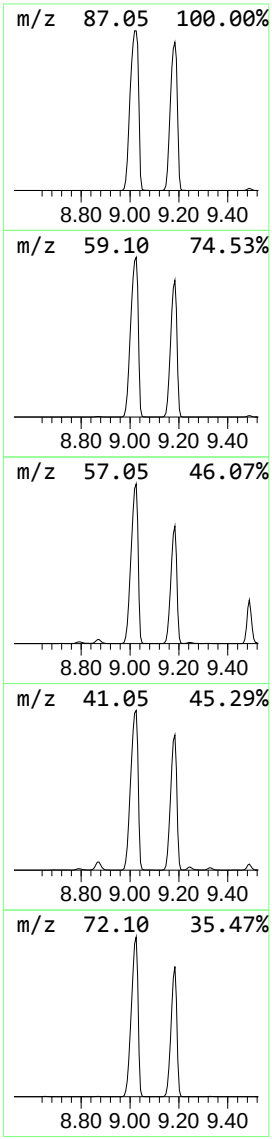
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.025	266.51 ug/l	81425900	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	72
2	Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	64
3	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	64
4	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	59
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	43





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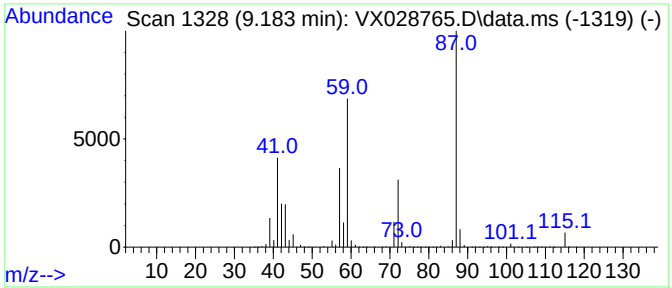
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

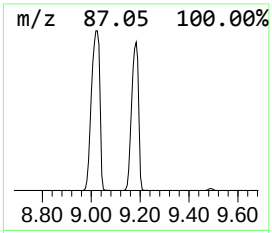
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

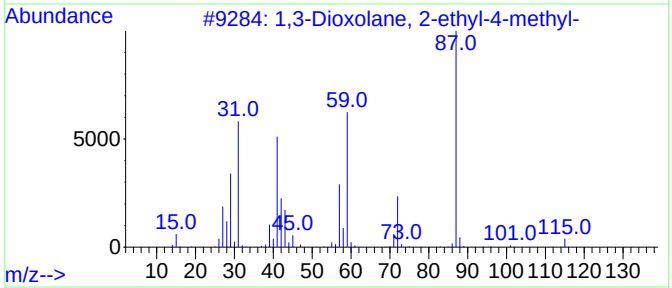
****
Peak Number 7 Oxazolidin-2-one Concentration Rank 6

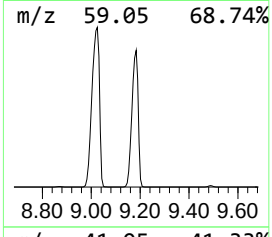
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.183	183.44 ug/l	56046800	Chlorobenzene-d5	10.055

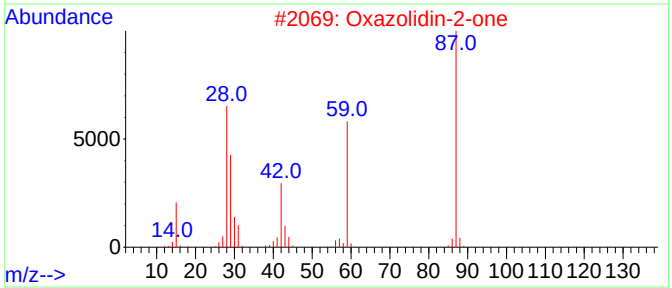
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	91
2	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	59
3	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	53
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	50
5	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	50

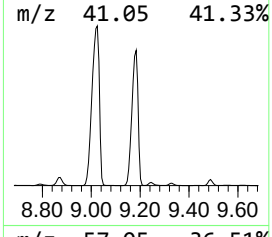


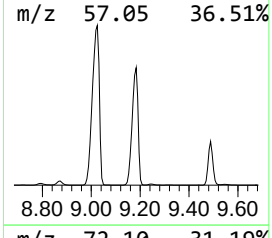


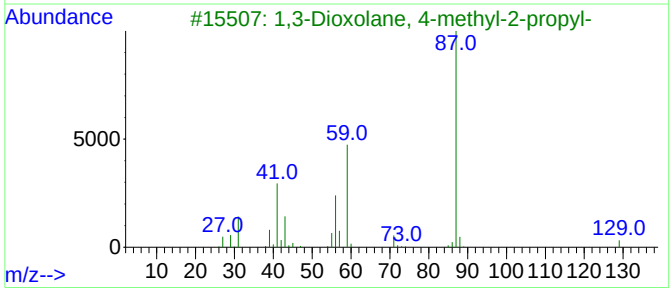


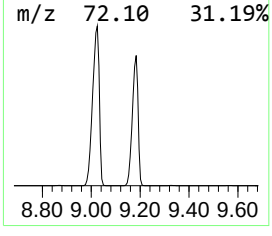












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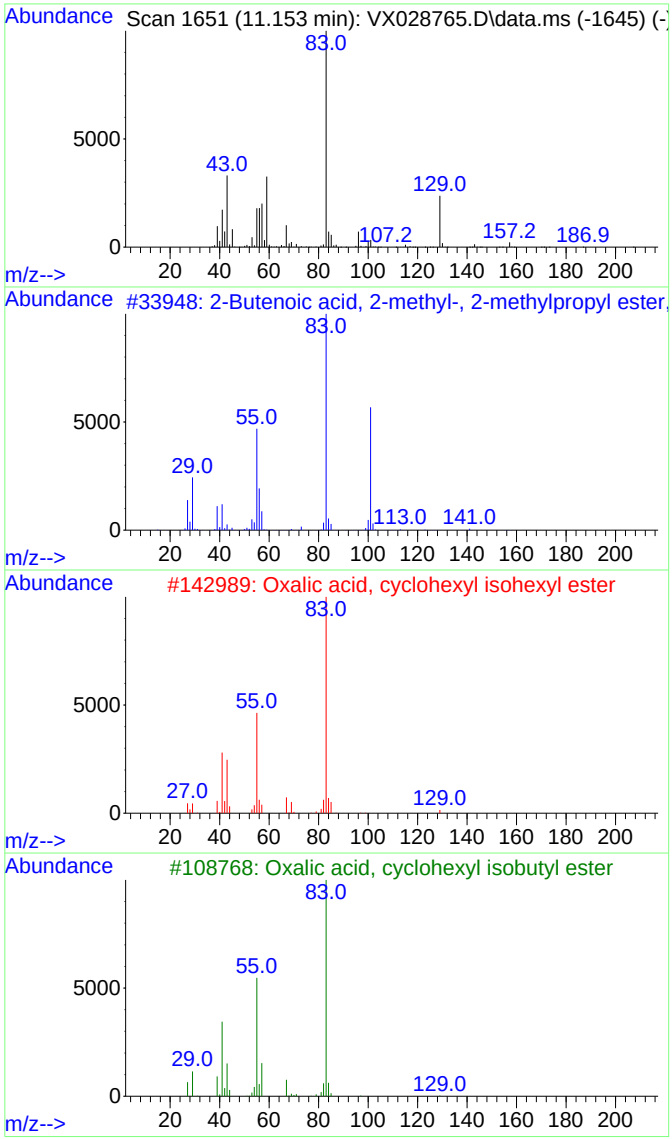
Quant Title : SW846 8260

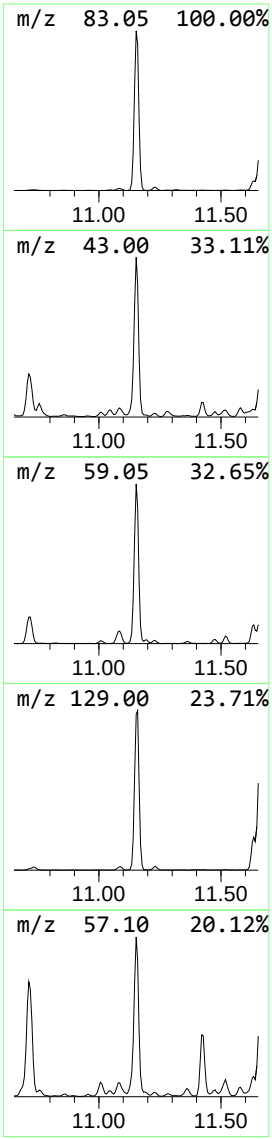
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 unknown11.153 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.153	104.83 ug/l	3789800	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenoic acid, 2-methyl-, 2-me...	156	C9H16O2	061692-84-0	47
2	Oxalic acid, cyclohexyl isohexyl...	256	C14H24O4	1010309-30-7	40
3	Oxalic acid, cyclohexyl isobutyl...	228	C12H20O4	1000309-30-4	40
4	1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	39
5	2-(1-Phenylethyl)-6-isopropyl-1,...	234	C15H22O2	1000431-40-0	36





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Operator : JC/MD
Sample : N2884-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31517

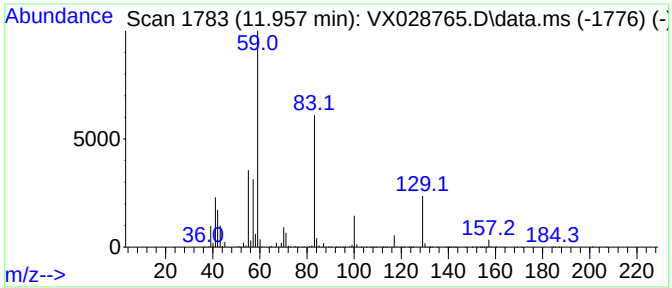
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

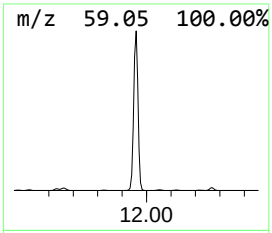
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

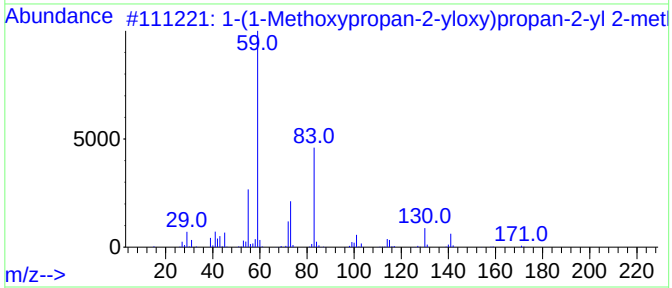
****
Peak Number 9 unknown11.957 Concentration Rank 4

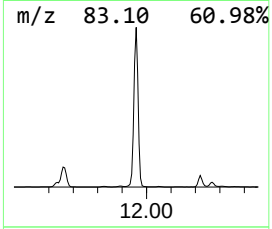
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.957	349.48 ug/l	12634200	1,4-Dichlorobenzene-d4	12.024

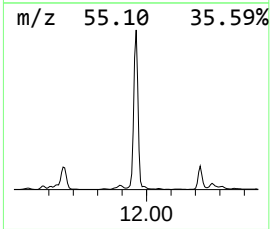
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(1-Methoxypropan-2-yloxy)propa...	230	C12H22O4	1000367-11-3	42
2	4,8,12,16-tetraoxaeicosan-1-ol	306	C16H34O5	1010397-63-6	38
3	3-Heptanol, 6-methyl-	130	C8H18O	018720-66-6	33
4	Acetaldoxime	59	C2H5NO	000107-29-9	32
5	Pentane, 3-ethoxy-	116	C7H16O	036749-13-0	32

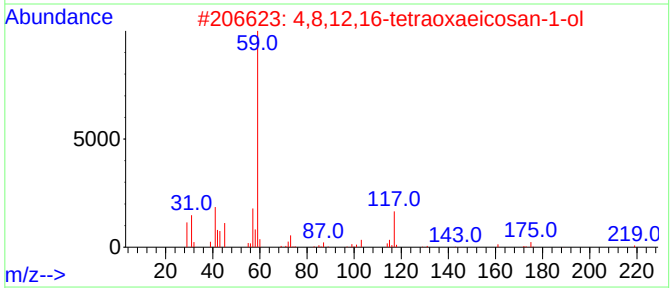


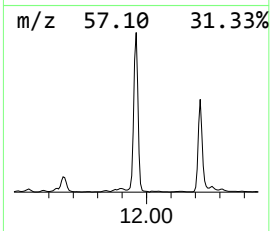


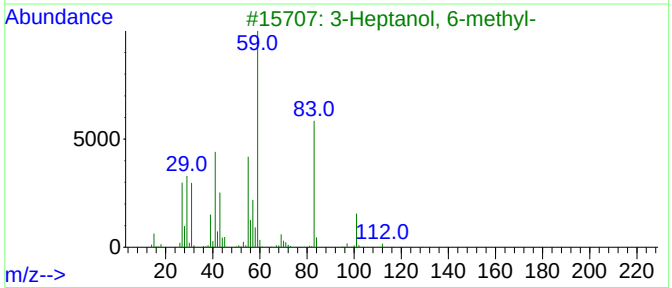


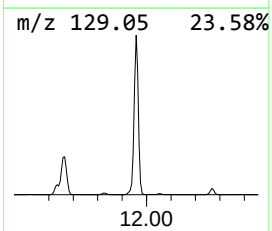












Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028765.D
Acq On : 17 May 2022 18:05
Operator : JC/MD
Sample : N2884-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31517

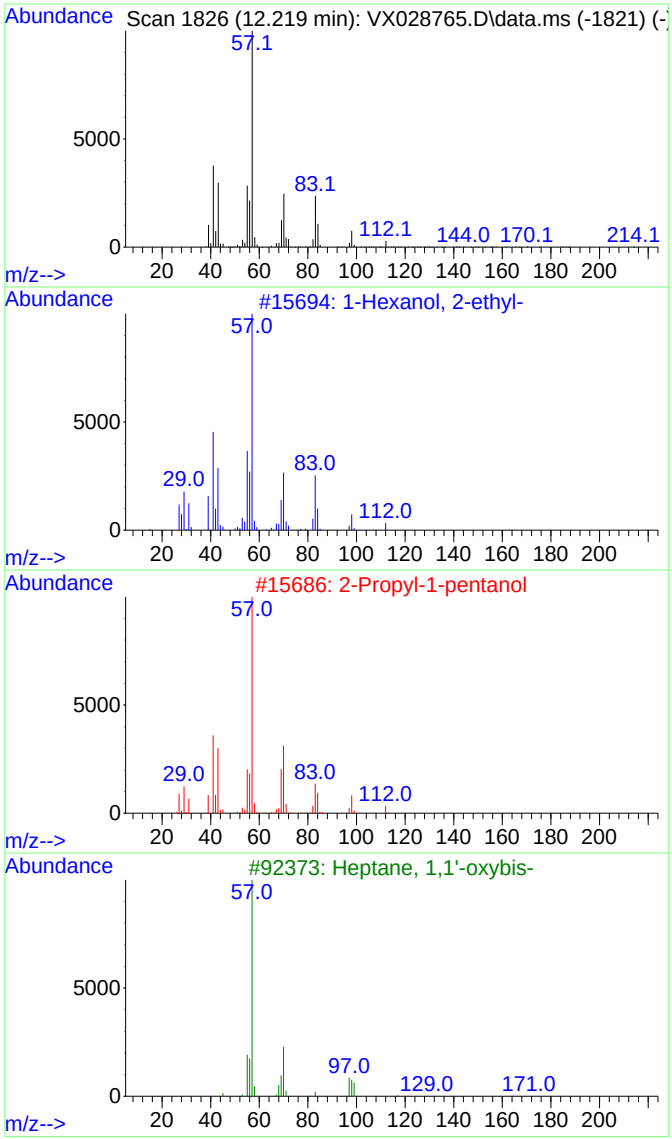
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.M
Quant Title : SW846 8260

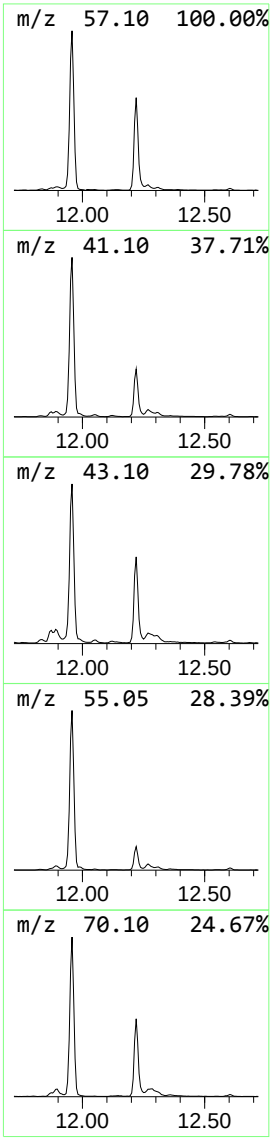
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	58.38 ug/l	2110580	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
5	Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051722\
Data File : VX028765.D
Acq On : 17 May 2022 18:05
Operator : JC/MD
Sample : N2884-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31517

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051222W.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
Acetaldehyde	1.447	514.6	ug/l	13001900	1	5.562	1263280	50.0
Propanal	2.288	2777.9	ug/l	70185900	1	5.562	1263280	50.0
1-Propanol	4.117	4450.1	ug/l	112435000	1	5.562	1263280	50.0
Butanal	4.270	101.7	ug/l	2569010	1	5.562	1263280	50.0
1,3-Dioxane, 2-...	6.885	57.1	ug/l	1998660	2	6.769	1749050	50.0
1,3-Dioxolane, ...	9.025	266.5	ug/l	81425900	3	10.055	15276500	50.0
Oxazolidin-2-one	9.183	183.4	ug/l	56046800	3	10.055	15276500	50.0
unknown11.153	11.153	104.8	ug/l	3789800	4	12.024	1807570	50.0
unknown11.957	11.957	349.5	ug/l	12634200	4	12.024	1807570	50.0
1-Hexanol, 2-et...	12.219	58.4	ug/l	2110580	4	12.024	1807570	50.0