LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011922\
Data File : VX026519.D
Acq On : 19 Jan 2022 15:10
Operator : JC/MD
Sample : N1187-06 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31282

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\82X011122W.M
Title : SW846 8260

Signal : TIC: VX026519.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.362	41	45	56	rVB	36163	46066	2.21%	0.645%
2	1.459	56	61	71	rVB	71569	87416	4.20%	1.224%
3	2.386	206	213	230	rBV	153074	265613	12.77%	3.721%
4	2.563	234	242	257	rBV2	15127	54868	2.64%	0.769%
5	5.391	695	706	720	rBV	84532	241082	11.59%	3.377%
6	5.556	720	733	749	rVB	147022	413006	19.86%	5.785%
7	5.958	788	799	811	rBV	97395	251568	12.10%	3.524%
8	6.763	921	931	942	rBV	226612	539259	25.93%	7.554%
9	6.879	942	950	963	rVB	16072	38396	1.85%	0.538%
10	7.214	997	1005	1013	rBV2	9262	21013	1.01%	0.294%
11	7.458	1038	1045	1051	rBV	37430	73275	3.52%	1.026%
12	7.531	1051	1057	1065	rVB	46125	88384	4.25%	1.238%
13	7.824	1098	1105	1113	rBV	11899	23233	1.12%	0.325%
14	8.653	1234	1241	1249	rBV	449249	708942	34.08%	9.931%
15	8.732	1249	1254	1268	rVB	47158	78147	3.76%	1.095%
16	8.964	1285	1292	1301	rBV	18309	34334	1.65%	0.481%
17	9.531	1379	1385	1407	rBV	305587	467185	22.46%	6.544%
18	10.055	1465	1471	1483	rBV	458557	602300	28.96%	8.437%
19	10.311	1507	1513	1525	rBV	1507942	2079929	100.00%	29.135%
20	11.079	1634	1639	1646	rBV	343792	438106	21.06%	6.137%
21	11.152	1646	1651	1659	rVB	53544	65570	3.15%	0.918%
22	12.024	1789	1794	1803	rVB	416423	521342	25.07%	7.303%

Sum of corrected areas: 7139034

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011922\
Data File : VX026519.D
Acq On : 19 Jan 2022 15:10
Operator : JC/MD
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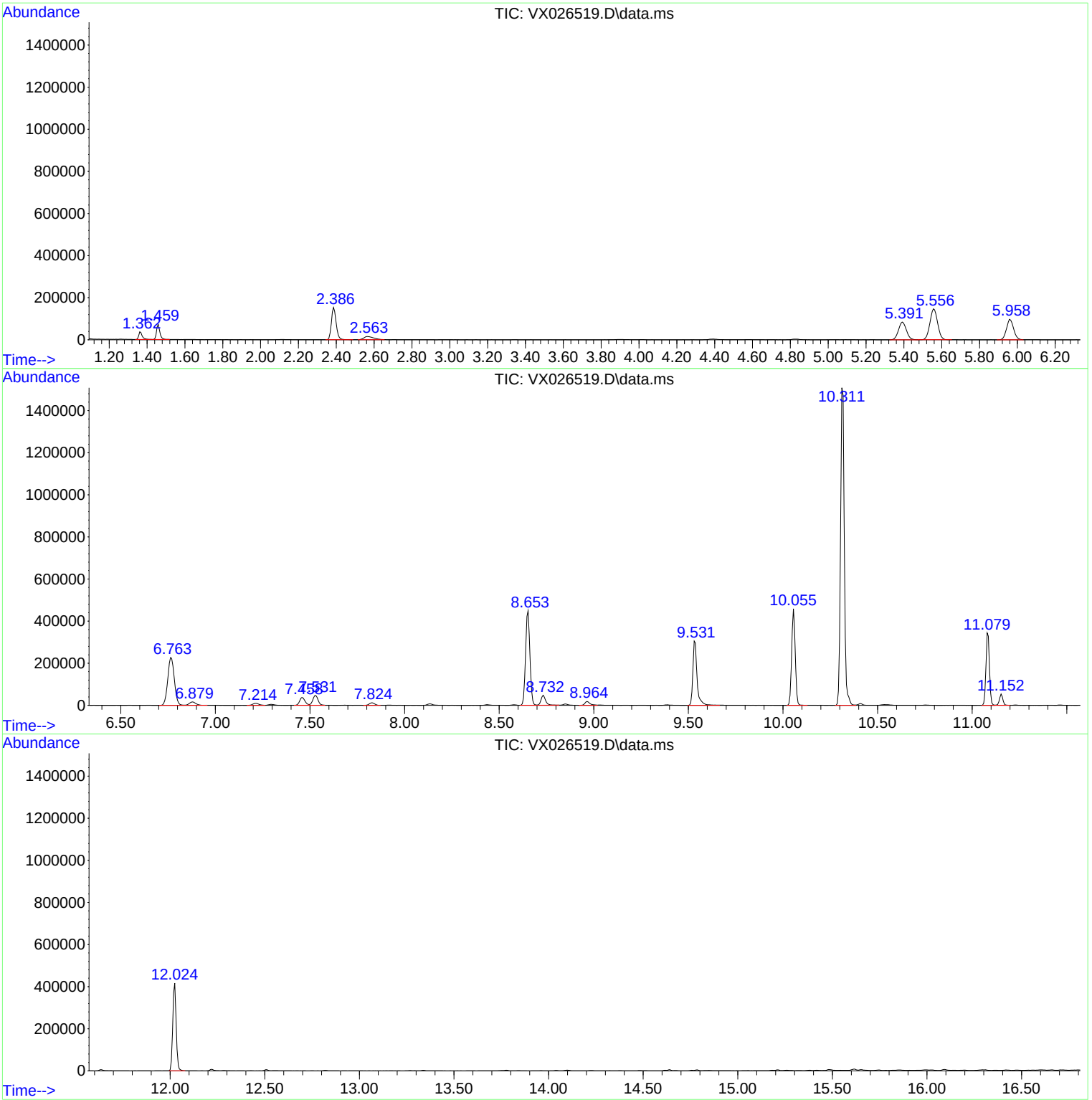
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31282

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011922\
Data File : VX026519.D
Acq On : 19 Jan 2022 15:10
Operator : JC/MD
Sample : N1187-06 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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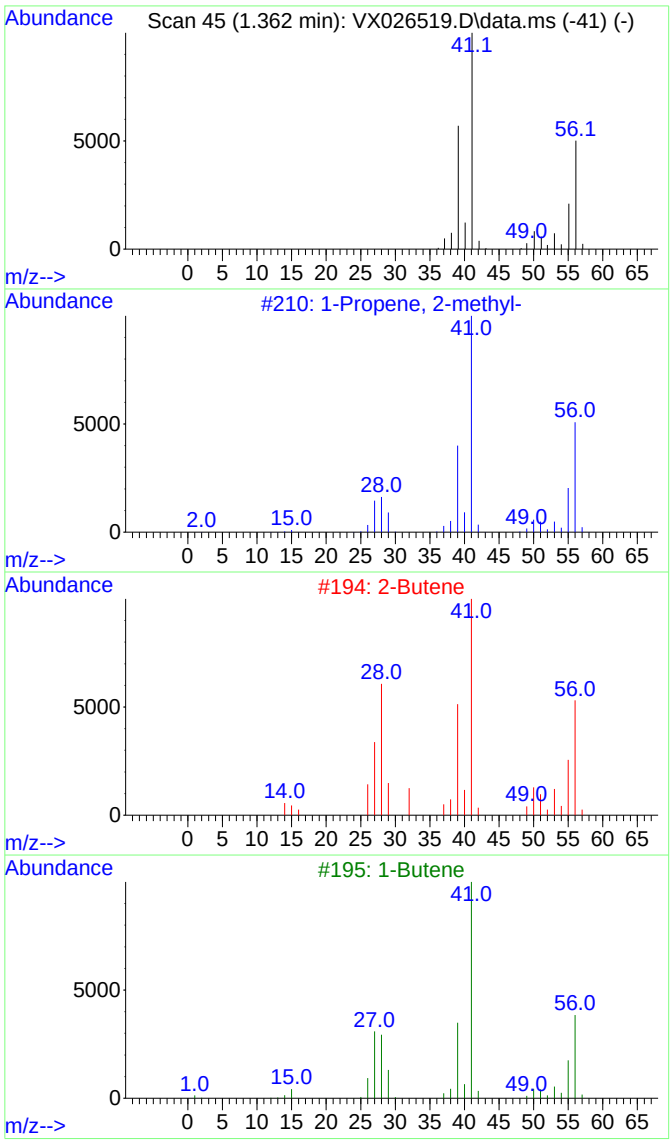
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

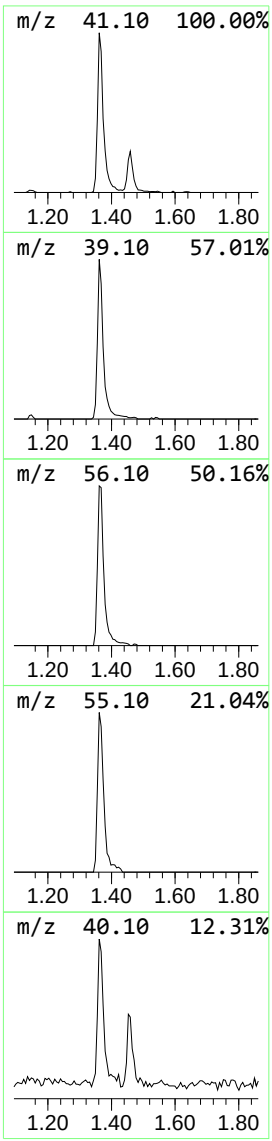
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1-Propene, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.362	5.58 ug/l	46066	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-	56	C4H8	000115-11-7	90
2	2-Butene	56	C4H8	000107-01-7	80
3	1-Butene	56	C4H8	000106-98-9	49
4	2-Butene, (Z)-	56	C4H8	000590-18-1	49
5	Cyclobutane	56	C4H8	000287-23-0	49





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011922\
Data File : VX026519.D
Acq On : 19 Jan 2022 15:10
Operator : JC/MD
Sample : N1187-06 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31282

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

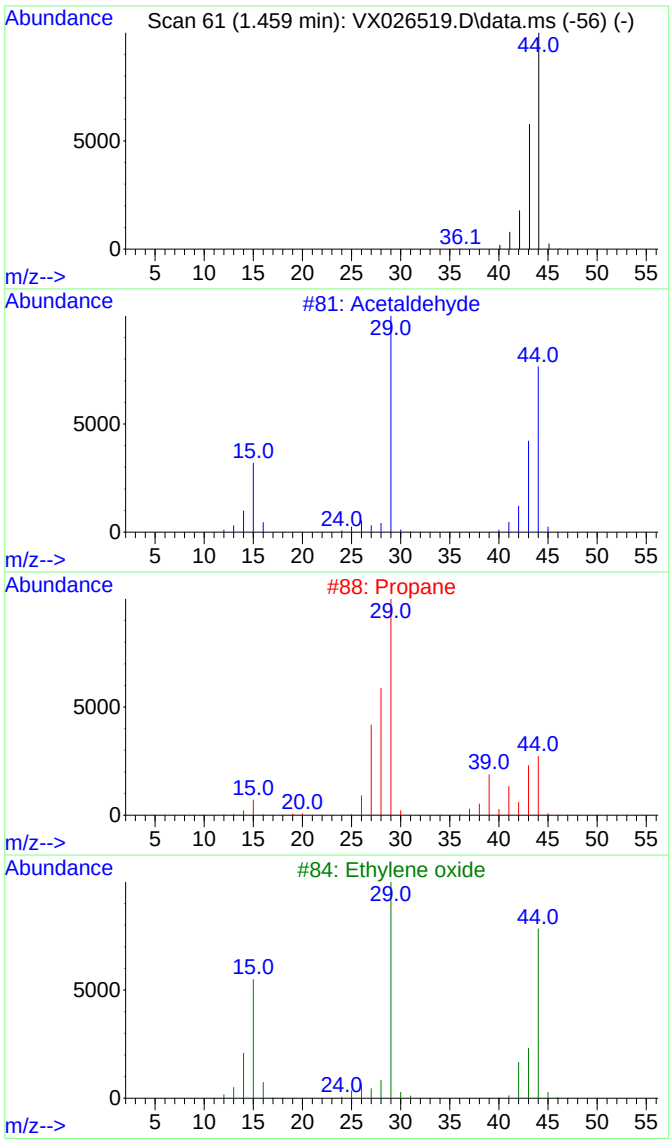
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

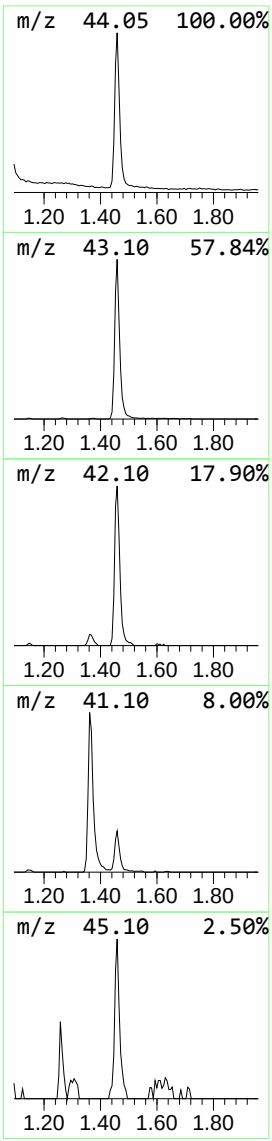
****

Peak Number 2 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.459	10.58 ug/l	87416	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	74
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Hydrogen isocyanate	43	CHNO	000075-13-8	3
5	Carbon dioxide	44	CO2	000124-38-9	3





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Data File : VX026519.D
Acq On : 19 Jan 2022 15:10
Operator : JC/MD
Sample : N1187-06 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31282

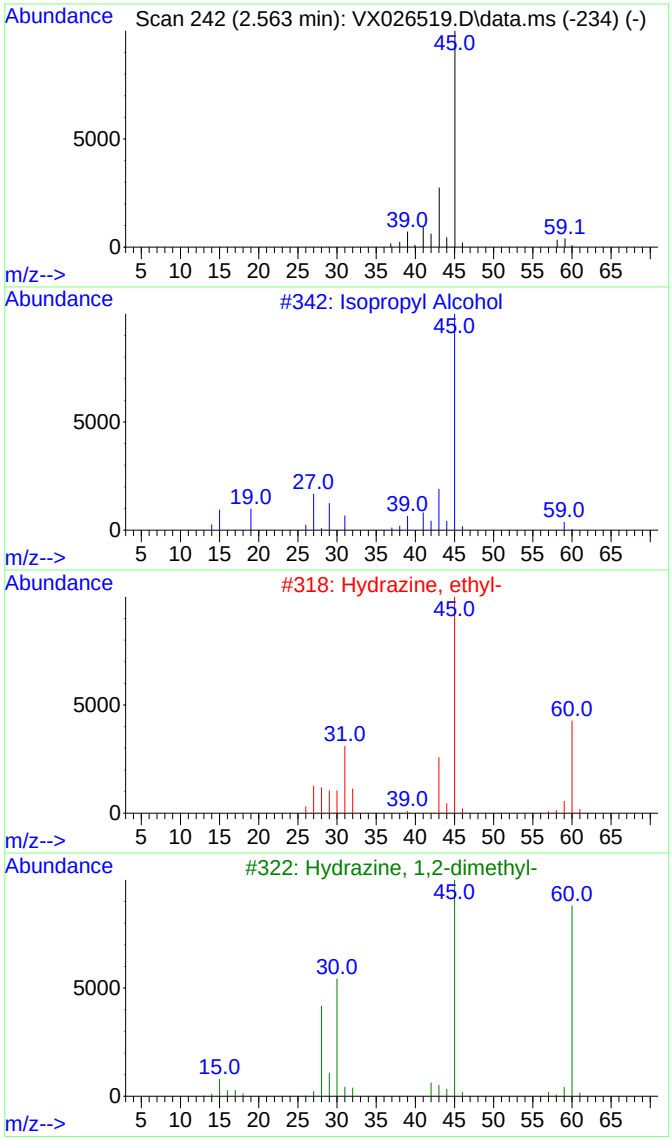
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

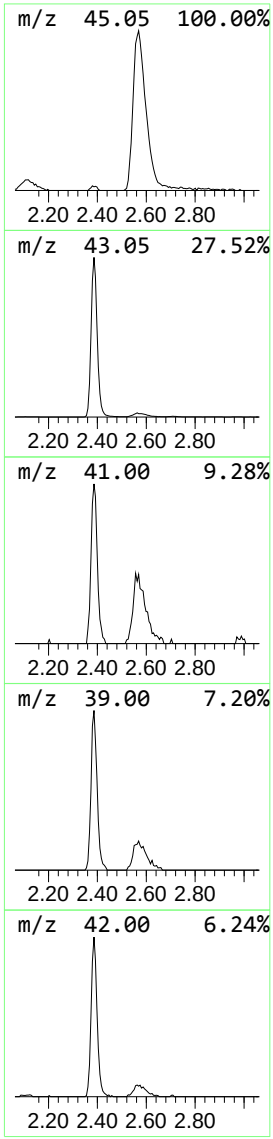
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Isopropyl Alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.563	6.64 ug/l	54868	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	83
2	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9
3	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4	Oxirane, (methoxymethyl)-	88	C4H8O2	000930-37-0	4
5	Formamide	45	CH3NO	000075-12-7	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011922\
Data File : VX026519.D
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Operator : JC/MD
Sample : N1187-06 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31282

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

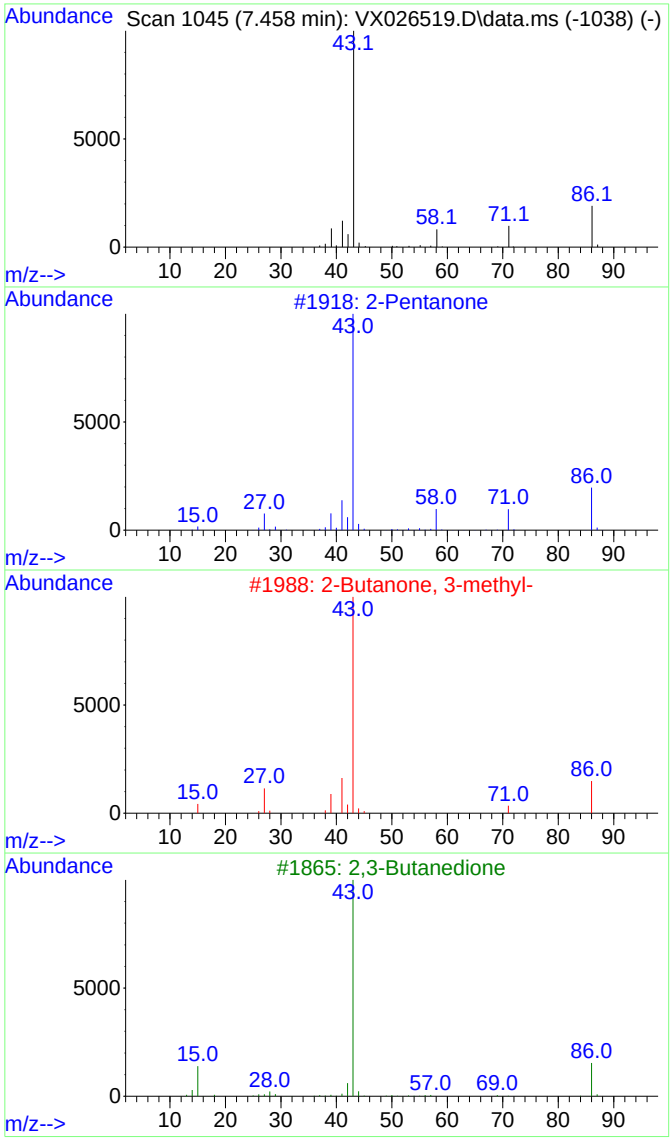
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

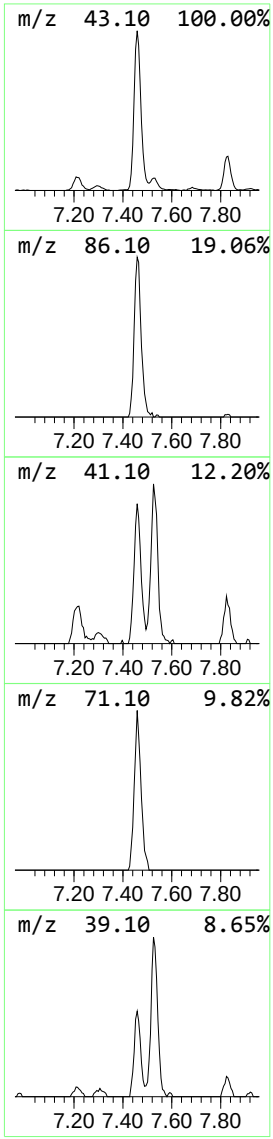
****

Peak Number 4 2-Pentanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.458	6.79 ug/l	73275	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	91
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	59
3	2,3-Butanedione	86	C4H6O2	000431-03-8	50
4	2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	9
5	Propane, 2-(ethenyloxy)-	86	C5H10O	000926-65-8	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011922\
Data File : VX026519.D
Acq On : 19 Jan 2022 15:10
Operator : JC/MD
Sample : N1187-06 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31282

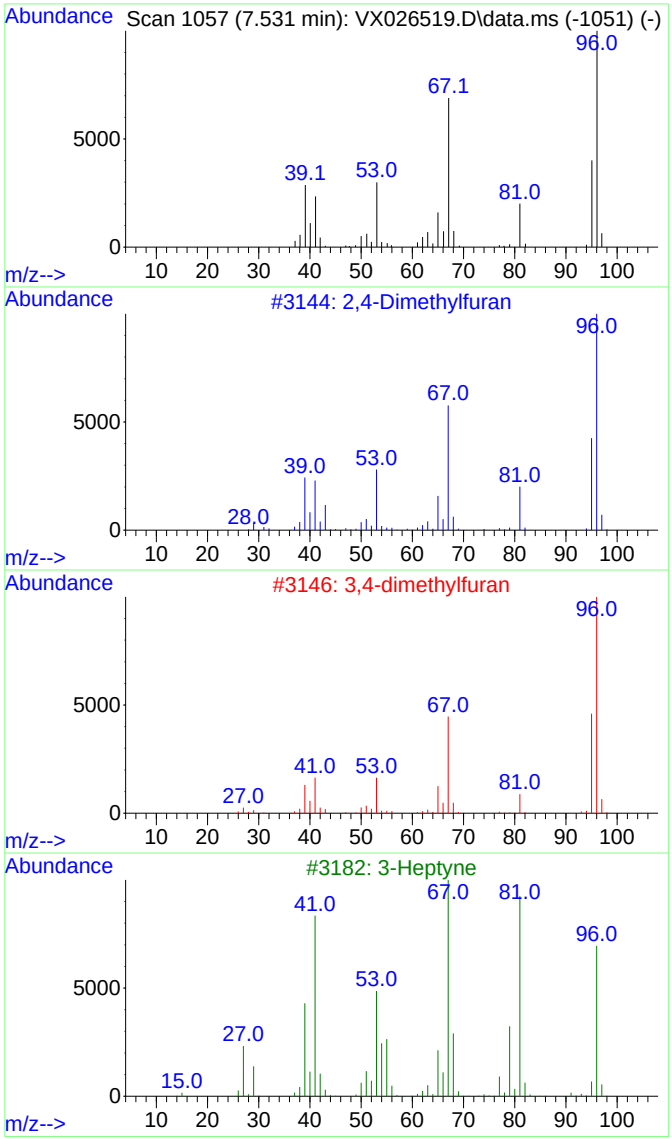
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

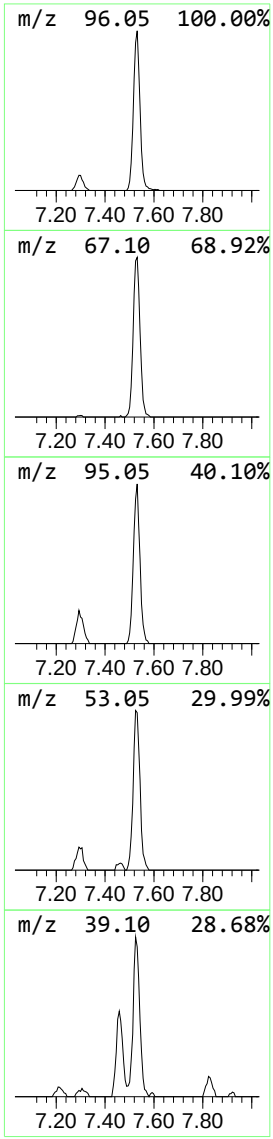
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2,4-Dimethylfuran Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.531	8.19 ug/l	88384	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dimethylfuran	96	C6H8O	003710-43-8	96
2	3,4-dimethylfuran	96	C6H8O	1000458-50-4	94
3	3-Heptyne	96	C7H12	002586-89-2	59
4	1H-Imidazole-4-carboxaldehyde	96	C4H4N2O	003034-50-2	53
5	2,3-dimethylfuran	96	C6H8O	1000458-49-9	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011922\
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31282

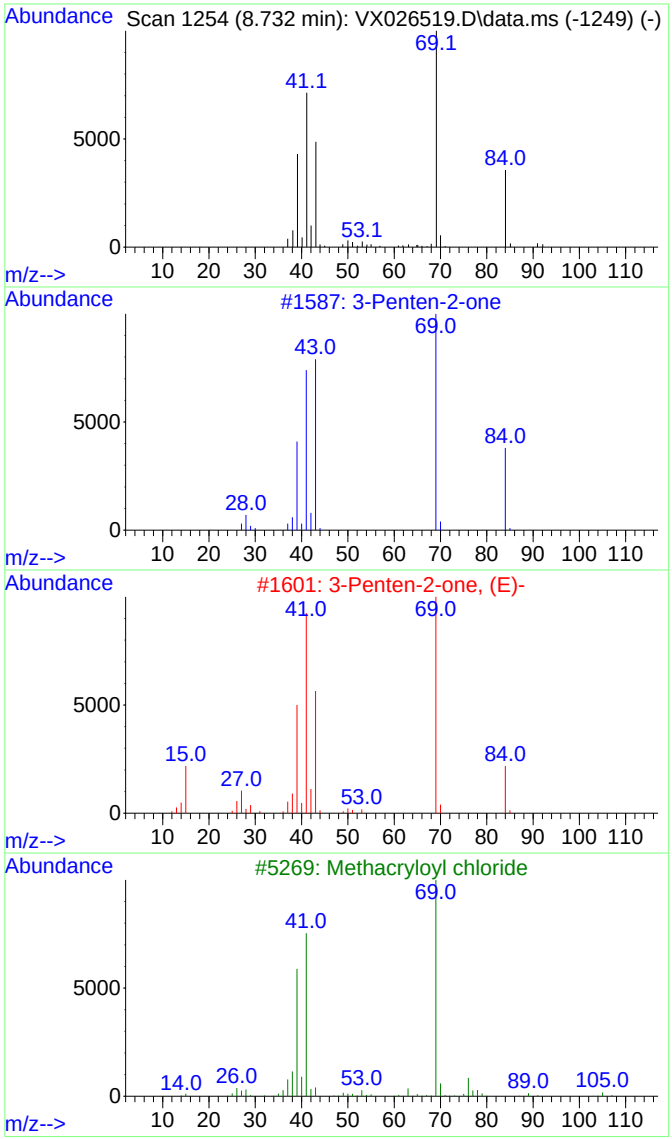
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

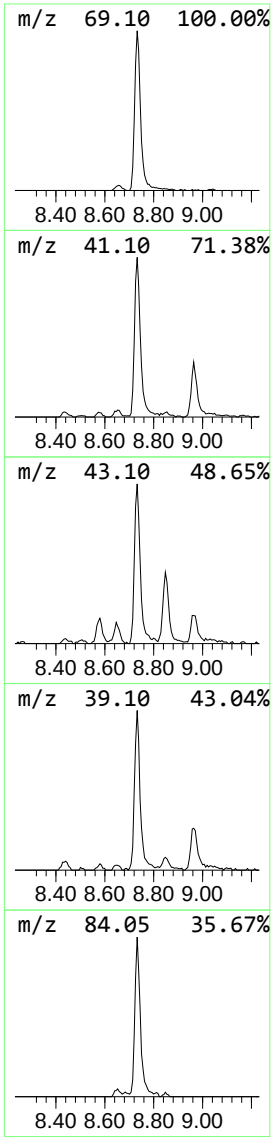
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 3-Penten-2-one Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.732	6.49 ug/l	78147	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one	84	C5H8O	000625-33-2	87
2	3-Penten-2-one, (E)-	84	C5H8O	003102-33-8	78
3	Methacryloyl chloride	104	C4H5ClO	000920-46-7	59
4	2-Butene, 2,3-dimethyl-	84	C6H12	000563-79-1	53
5	2-Butenoic acid, 4-nitrophenyl e...	207	C10H9NO4	014617-88-0	53





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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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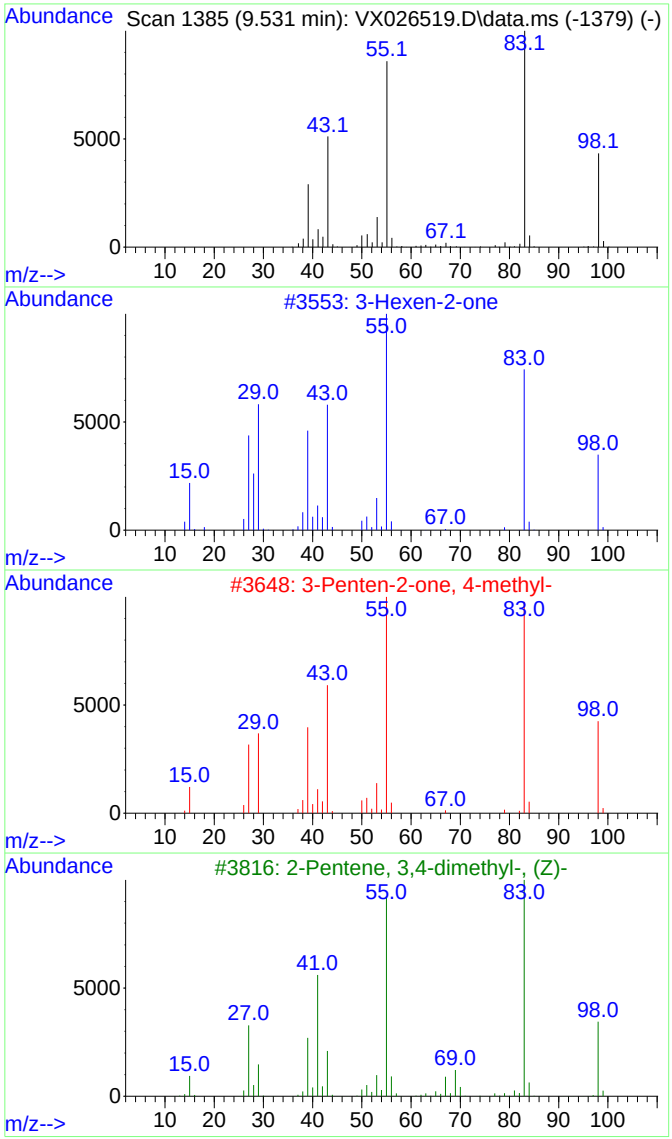
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

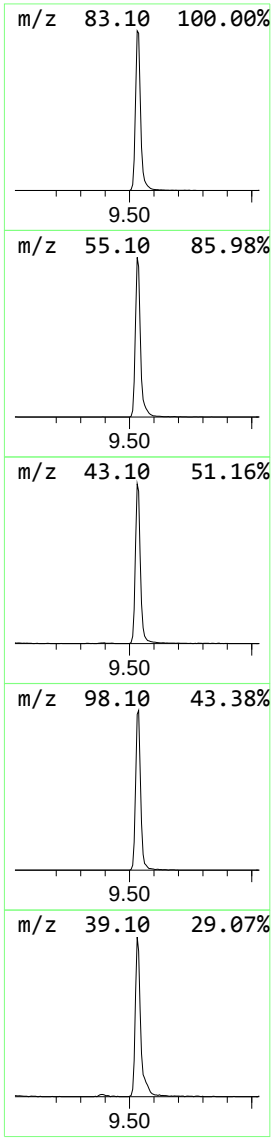
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.531	38.78 ug/l	467185	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5	2,4-Azetidinedione, 3,3-diethyl-	141	C7H11NO2	042282-85-9	78





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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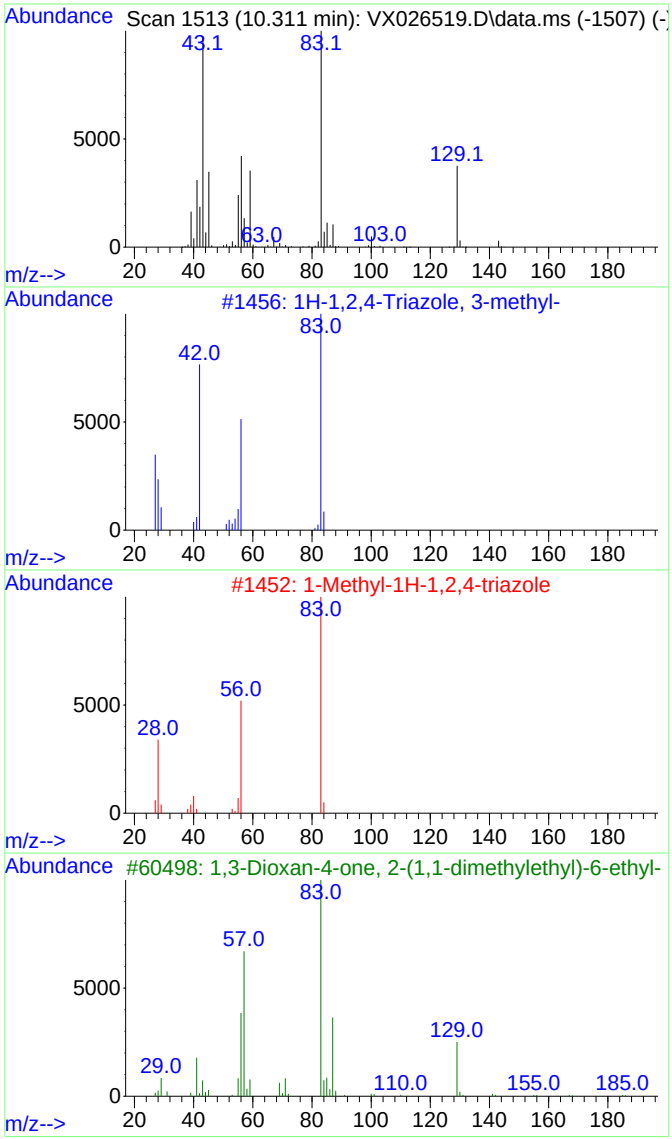
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.M
Quant Title : SW846 8260

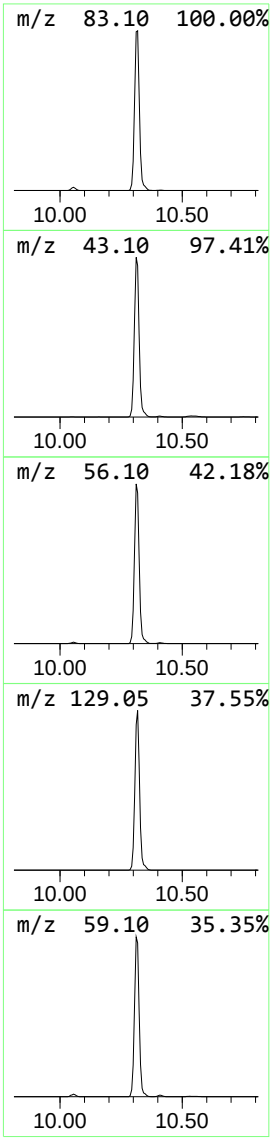
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 unknown10.311 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.311	172.67 ug/l	2079930	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-1,2,4-Triazole, 3-methyl-	83	C3H5N3	007170-01-6	43
2	1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	37
3	1,3-Dioxan-4-one, 2-(1,1-dimethy...	186	C10H18O3	113505-80-9	36
4	Oxalic acid, cyclohexyl butyl ester	228	C12H20O4	1000309-30-5	25
5	2,2-Dimethyl-4-pentenoic acid	128	C7H12O2	016386-93-9	25





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MSVOA_X
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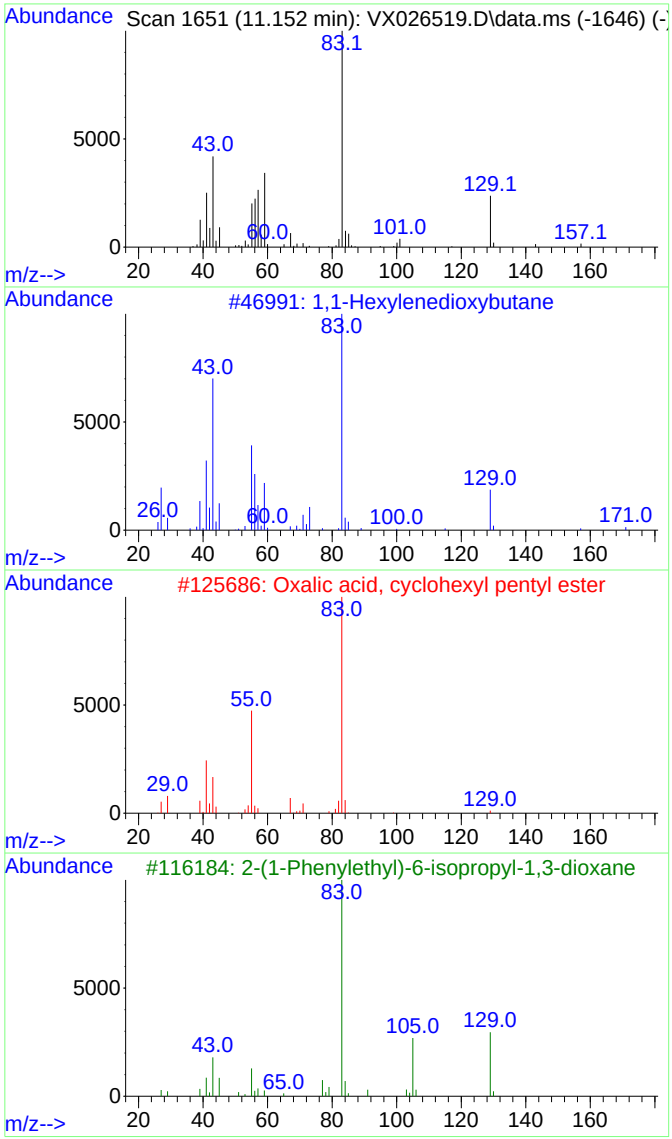
Quant Title : SW846 8260

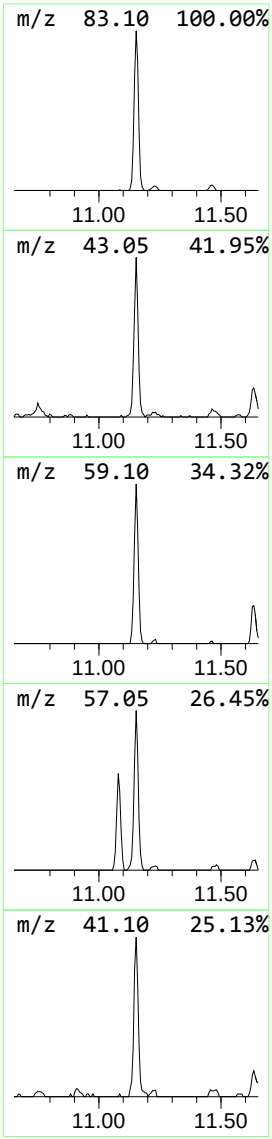
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1,1-Hexylenedioxybutane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.153	6.29 ug/l	65570	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	56
2	Oxalic acid, cyclohexyl pentyl e...	242	C13H22O4	1000309-30-6	37
3	2-(1-Phenylethyl)-6-isopropyl-1,...	234	C15H22O2	1000431-40-0	36
4	Hexanal ethyl trans-2-hexenyl ac...	228	C14H28O2	1000431-42-6	36
5	n-Butyl tiglate	156	C9H16O2	007785-66-2	33





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011922\
Data File : VX026519.D
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31282

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011122W.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
1-Propene, 2-me...	1.362	5.6	ug/l	46066	1	5.556	413006	50.0
Acetaldehyde	1.459	10.6	ug/l	87416	1	5.556	413006	50.0
Isopropyl Alcohol	2.563	6.6	ug/l	54868	1	5.556	413006	50.0
2-Pentanone	7.458	6.8	ug/l	73275	2	6.763	539259	50.0
2,4-Dimethylfuran	7.531	8.2	ug/l	88384	2	6.763	539259	50.0
3-Penten-2-one	8.732	6.5	ug/l	78147	3	10.055	602300	50.0
3-Hexen-2-one	9.531	38.8	ug/l	467185	3	10.055	602300	50.0
unknown10.311	10.311	172.7	ug/l	2079930	3	10.055	602300	50.0
1,1-Hexylenedio...	11.153	6.3	ug/l	65570	4	12.024	521342	50.0