LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052921\
Data File : VX022284.D
Acq On : 29 May 2021 04:38
Operator : JC/MD
Sample : M2517-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1917

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\82X051921W.M
Title : SW846 8260

Signal : TIC: VX022284.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.124	160	170	185	rBV3	18680	84030	3.12%	1.131%
2	2.398	207	215	227	rBV	66082	117771	4.37%	1.585%
3	4.580	565	573	584	rVB2	18890	52385	1.95%	0.705%
4	5.397	694	707	719	rBV2	48737	139682	5.19%	1.880%
5	5.562	723	734	748	rVB2	76960	213187	7.92%	2.870%
6	5.964	790	800	813	rBV2	60563	163631	6.08%	2.203%
7	6.769	923	932	943	rBV	138599	328739	12.21%	4.426%
8	7.135	978	992	1001	rVB5	12993	30181	1.12%	0.406%
9	8.580	1223	1229	1235	rBV	24705	38711	1.44%	0.521%
10	8.653	1235	1241	1249	rVV	300265	465072	17.27%	6.261%
11	10.055	1461	1471	1482	rBV	283980	396964	14.74%	5.344%
12	11.085	1635	1640	1646	rBV	224555	282131	10.48%	3.798%
13	11.841	1759	1764	1769	rBV	29064	34283	1.27%	0.462%
14	12.024	1789	1794	1802	rVB	287418	353833	13.14%	4.763%
15	12.219	1821	1826	1844	rBV	874970	1108877	41.18%	14.928%
16	12.591	1877	1887	1898	rBV3	26693	55672	2.07%	0.749%
17	12.859	1926	1931	1936	rBV	25403	32238	1.20%	0.434%
18	13.103	1968	1971	1974	rBV2	26570	35580	1.32%	0.479%
19	13.140	1975	1977	1987	rVB6	18288	35972	1.34%	0.484%
20	13.426	2019	2024	2044	rBV	2180811	2692936	100.00%	36.253%
21	13.695	2064	2068	2072	rBV3	19904	27681	1.03%	0.373%
22	13.896	2097	2101	2114	rVB3	18509	45618	1.69%	0.614%
23	14.201	2146	2151	2170	rBV	367701	618464	22.97%	8.326%
24	14.920	2265	2269	2281	rBV3	19238	39109	1.45%	0.526%
25	15.255	2320	2324	2334	rBV2	22019	35435	1.32%	0.477%

Sum of corrected areas: 7428182

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MSVOA_X
ClientSampleId :
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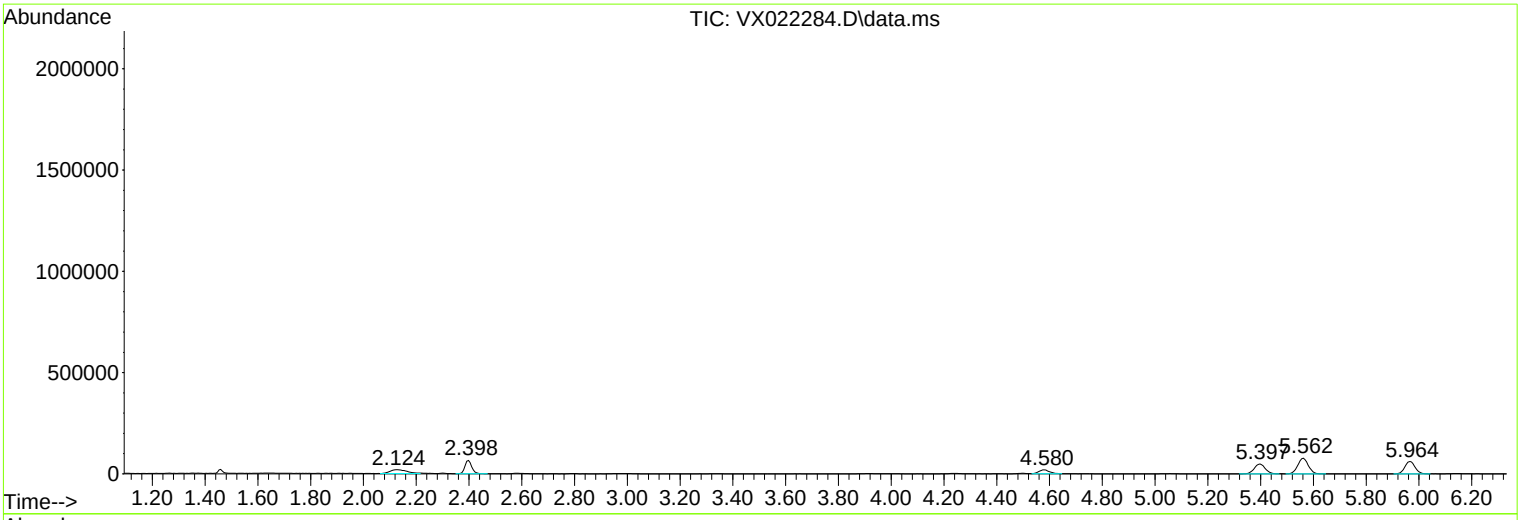
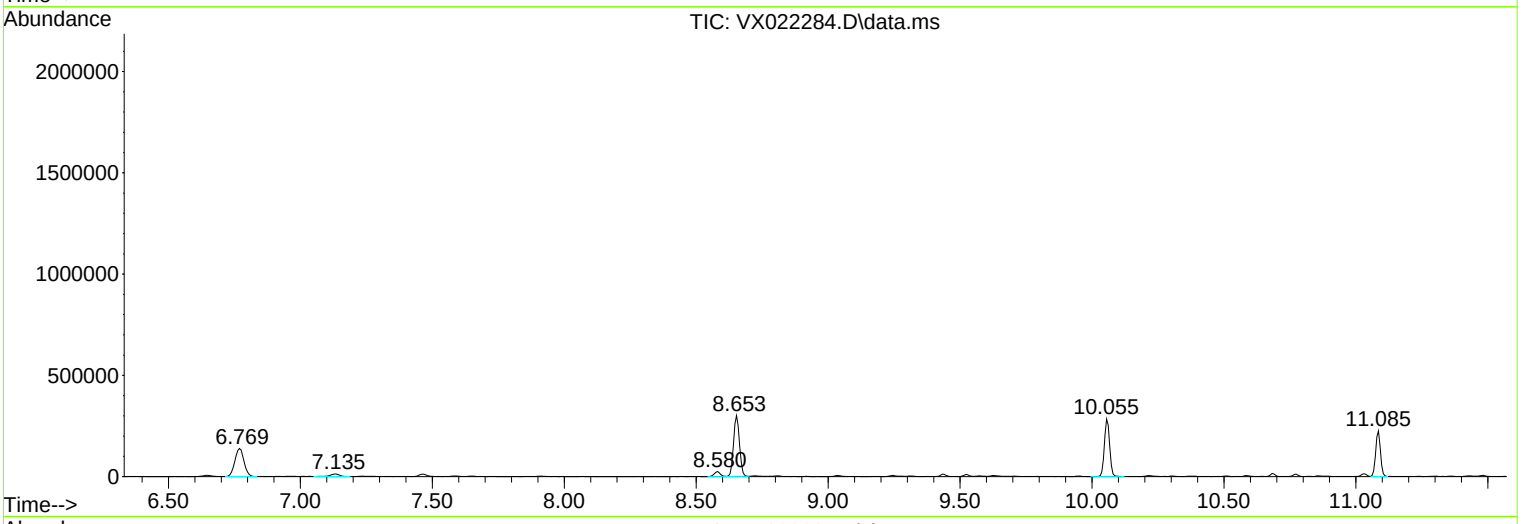
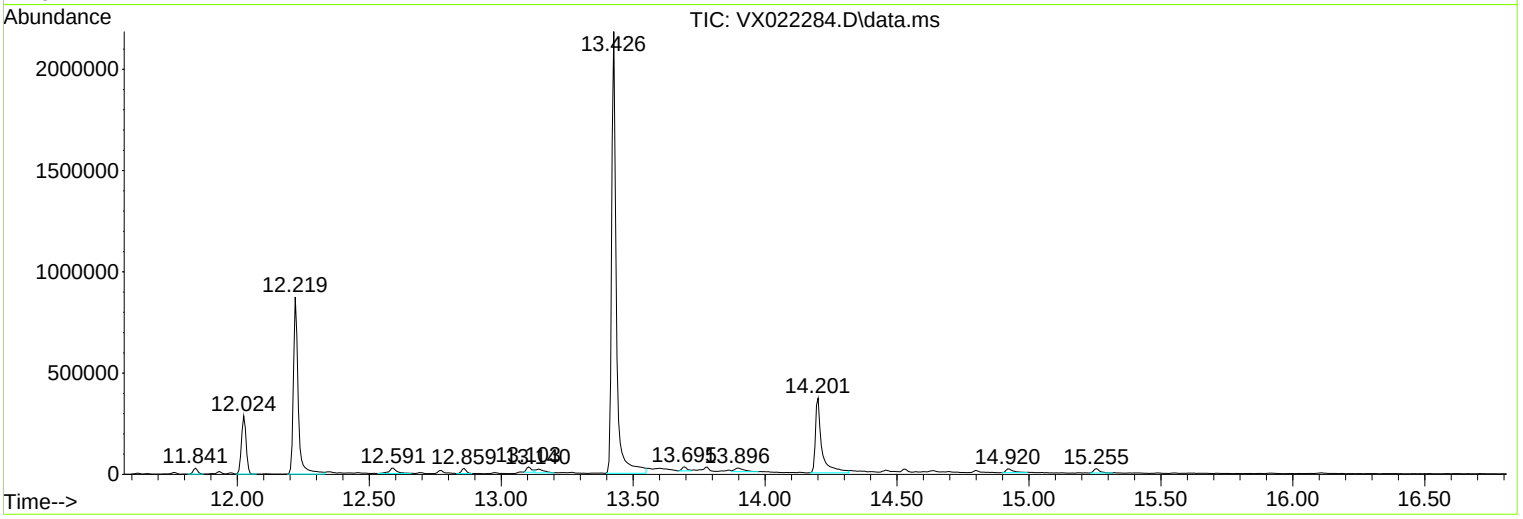
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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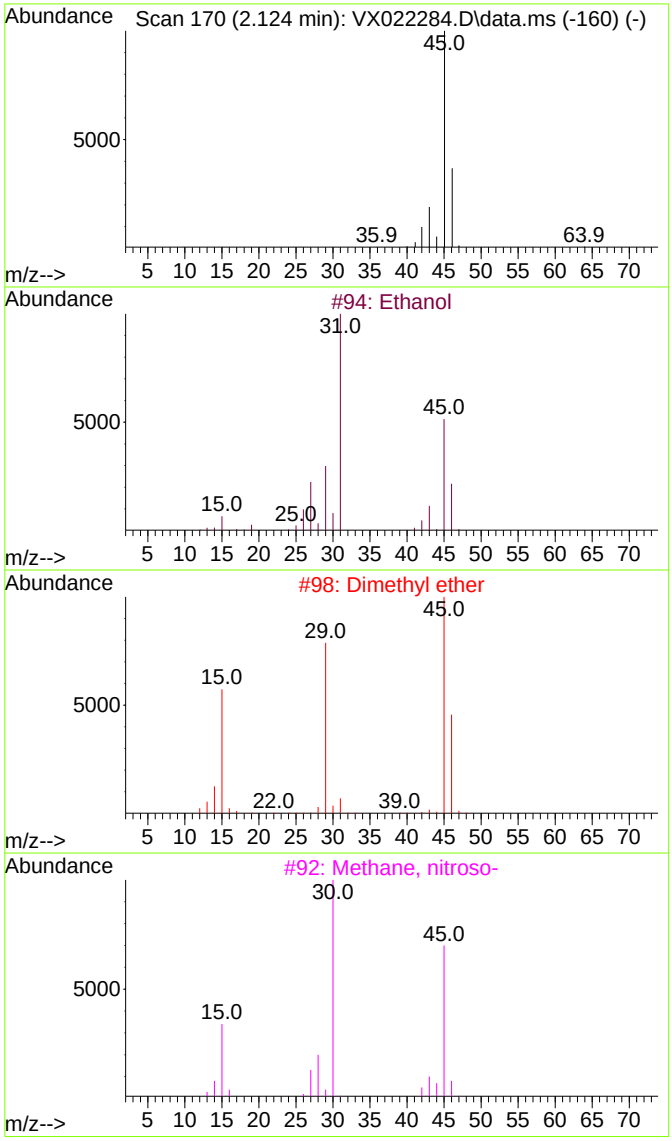
Quant Title : SW846 8260

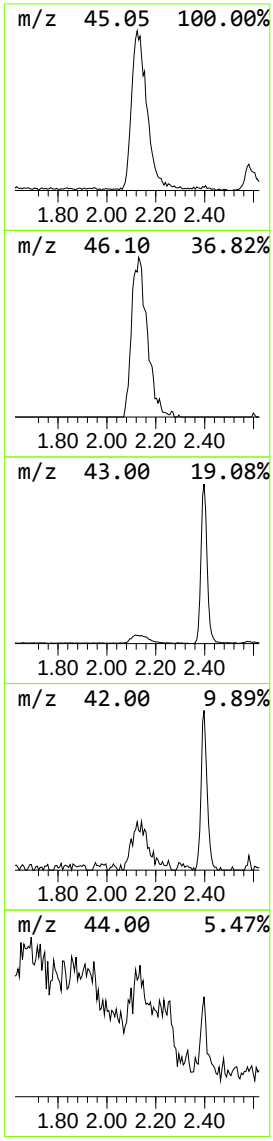
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.124	19.71 ug/l	84030	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	86
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	7
4	Formic acid	46	CH2O2	000064-18-6	4
5	Formamide	45	CH3NO	000075-12-7	3





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Operator : JC/MD
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ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1917

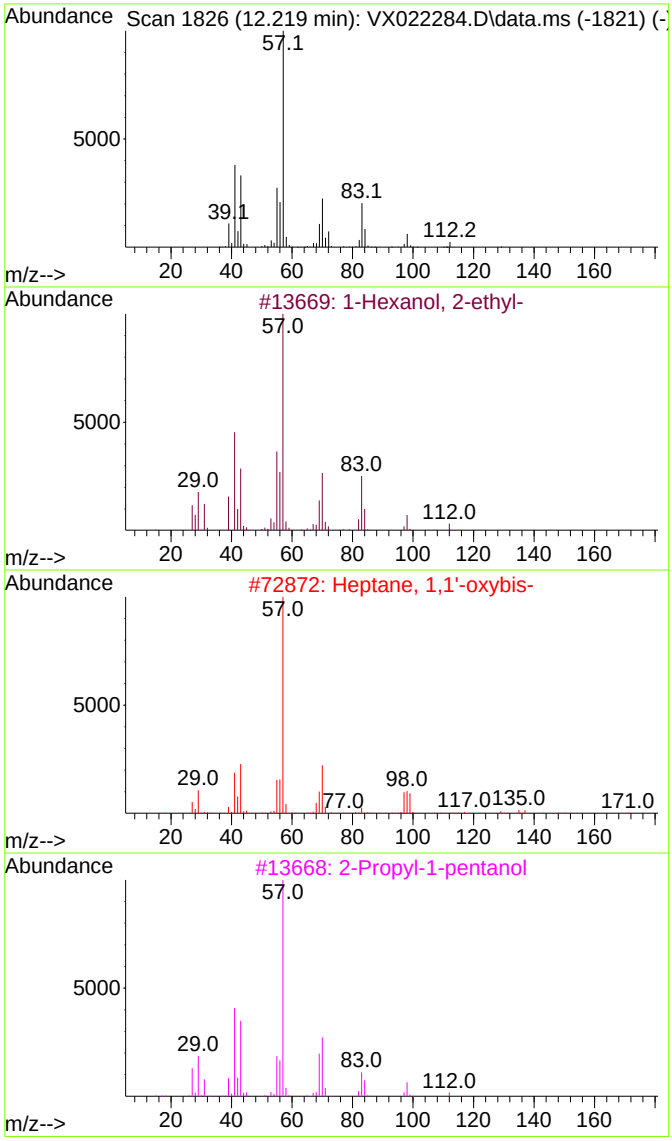
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

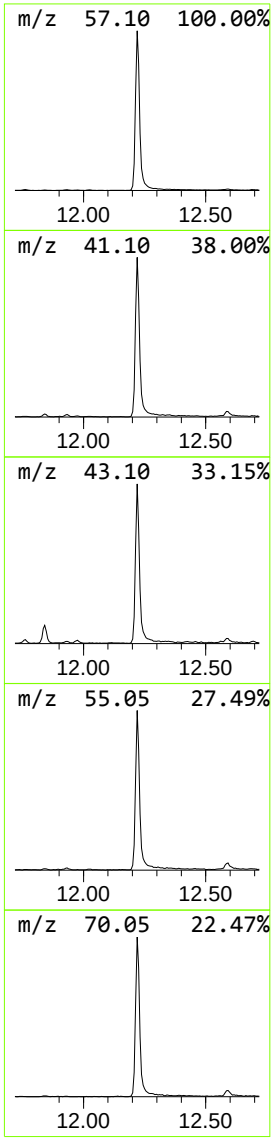
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	156.69 ug/l	1108880	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	78
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
5	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	43





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Operator : JC/MD
Sample : M2517-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1917

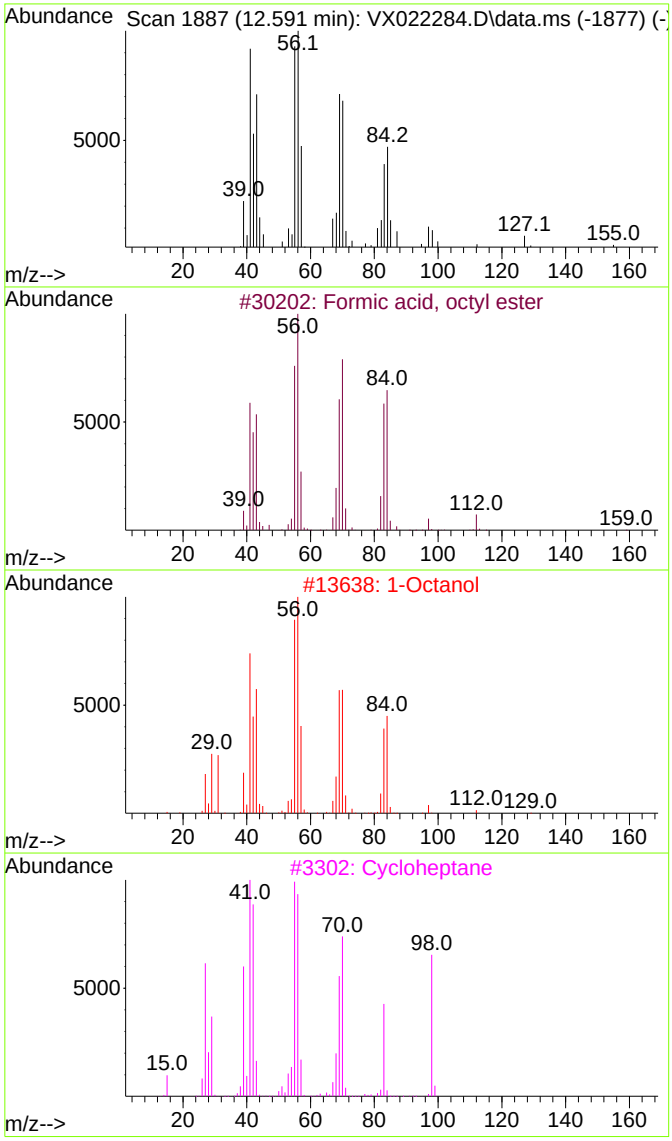
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

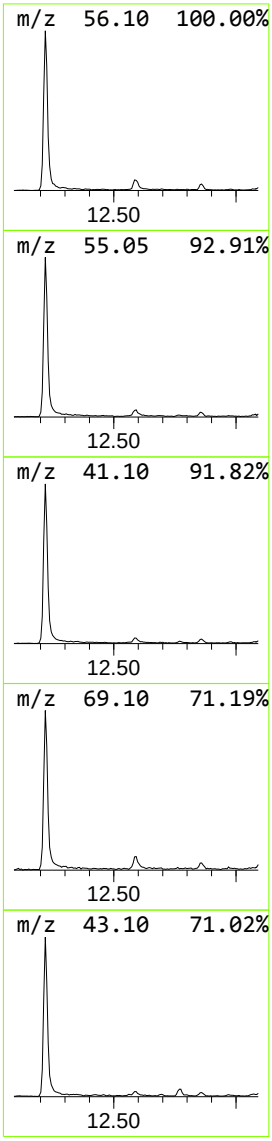
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Formic acid, octyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.591	7.87 ug/l	55672	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Formic acid, octyl ester	158	C9H18O2	000112-32-3	86
2	1-Octanol	130	C8H18O	000111-87-5	86
3	Cycloheptane	98	C7H14	000291-64-5	76
4	Cyclobutane, 1-butyl-2-ethyl-	140	C10H20	1000150-67-3	64
5	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	49





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Acq On : 29 May 2021 04:38
Operator : JC/MD
Sample : M2517-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1917

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

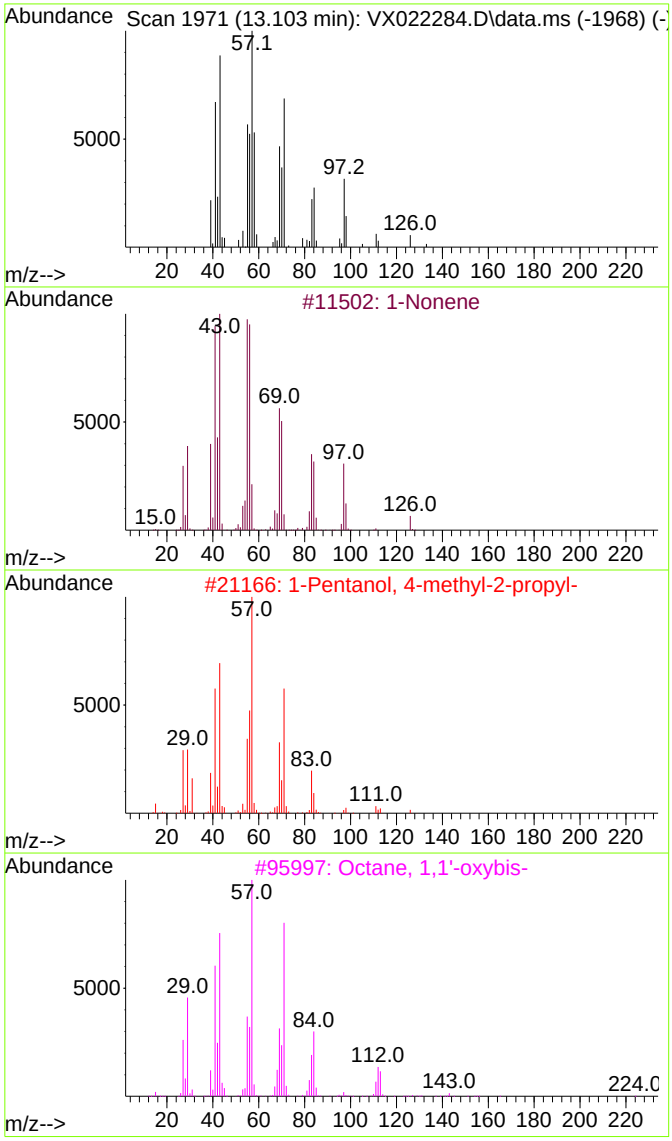
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

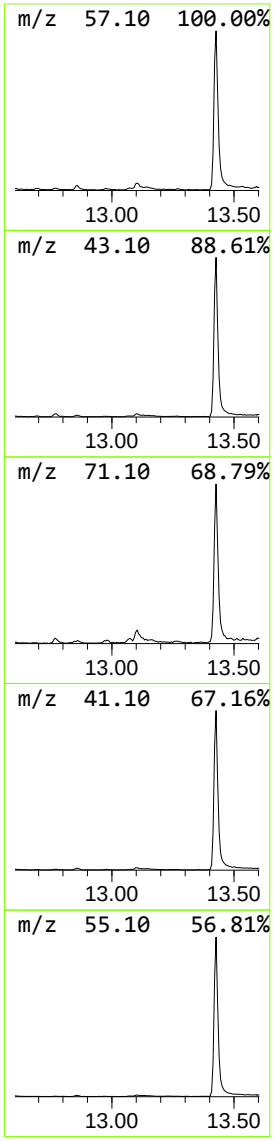
****

Peak Number 4 1-Nonene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.103	5.03 ug/l	35580	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonene	126	C9H18	000124-11-8	50
2	1-Pentanol, 4-methyl-2-propyl-	144	C9H20O	054004-41-0	47
3	Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	47
4	Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	38
5	Cycloheptane	98	C7H14	000291-64-5	35





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Operator : JC/MD
Sample : M2517-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1917

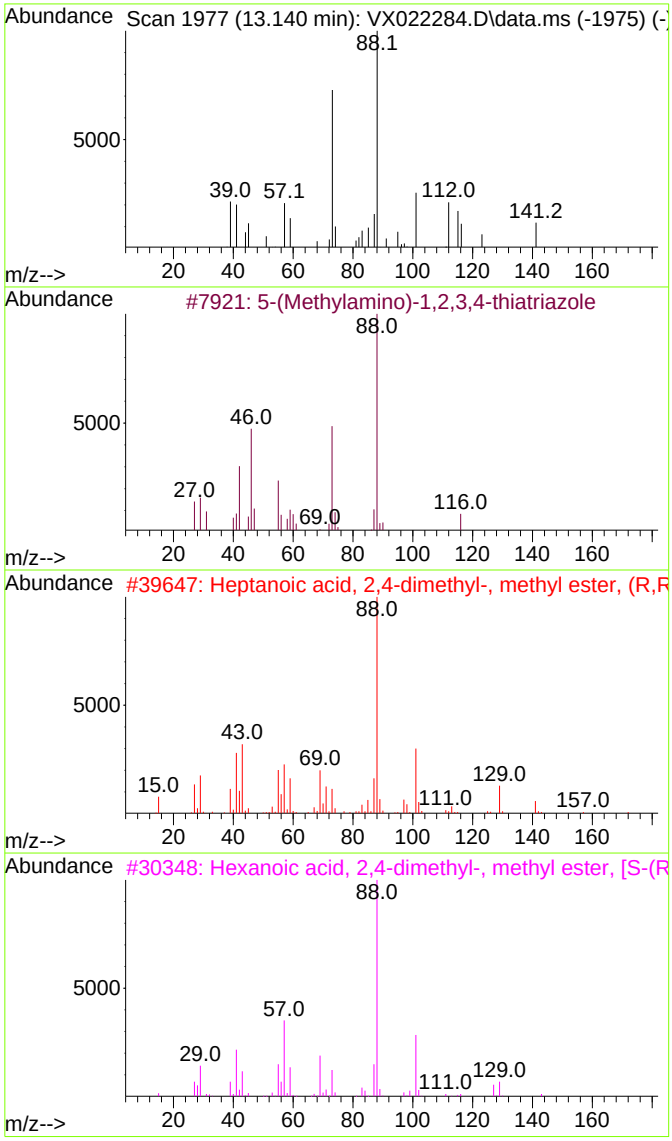
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

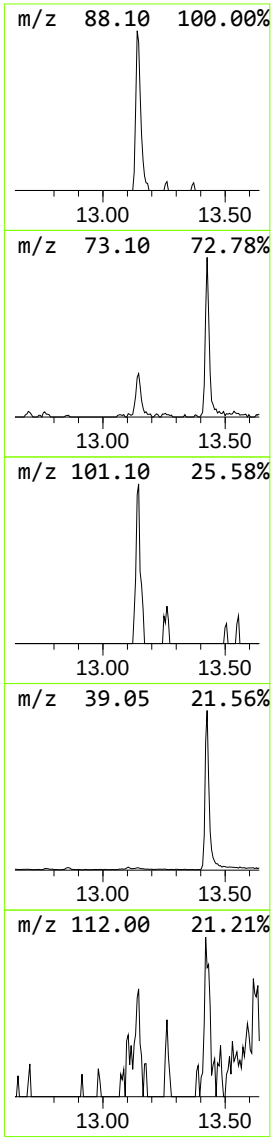
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 5-(Methylamino)-1,2,3,4-thi... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.140	5.08 ug/l	35972	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-(Methylamino)-1,2,3,4-thiatria...	116	C2H4N4S	052098-72-3	50
2	Heptanoic acid, 2,4-dimethyl-, m...	172	C10H20O2	018524-86-2	45
3	Hexanoic acid, 2,4-dimethyl-, me...	158	C9H18O2	014251-45-7	42
4	Methyl 2-methylhexanoate	144	C8H16O2	002177-81-3	36
5	Hexanoic acid, 2,4-dimethyl-, me...	158	C9H18O2	014251-44-6	36





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ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
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TIC Library : C:\DATABASE\NIST11.L
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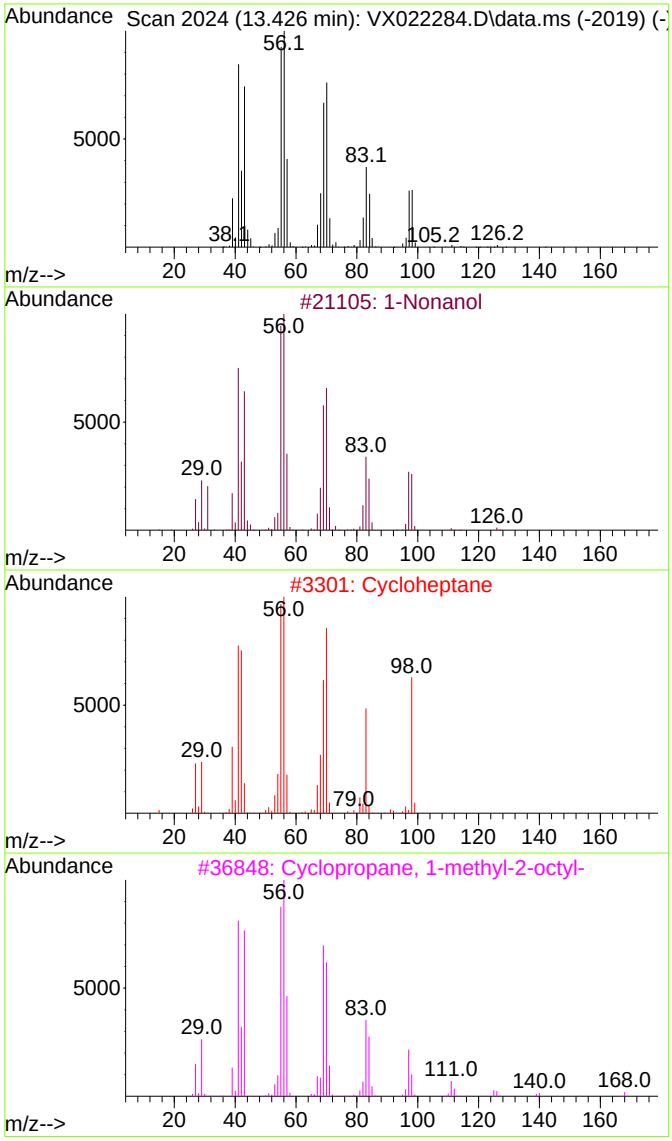
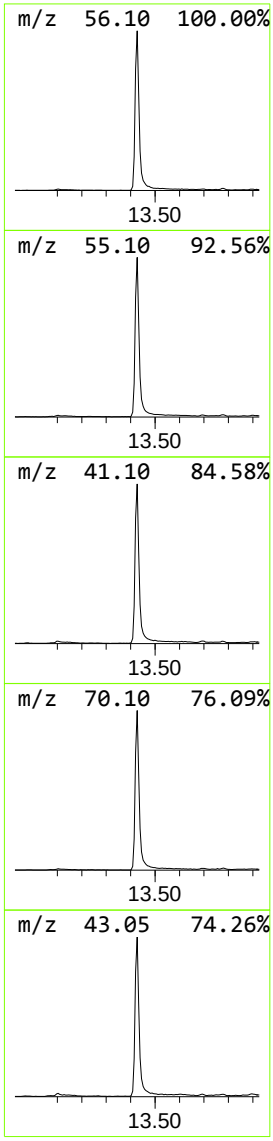
****
Peak Number 6 1-Nonanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	380.54 ug/l	2692940	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanol	144	C9H20O	000143-08-8	91
2	Cycloheptane	98	C7H14	000291-64-5	83
3	Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	80
4	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	68
5	Isopropylcyclobutane	98	C7H14	000872-56-0	68





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ALS Vial : 40 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1917

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

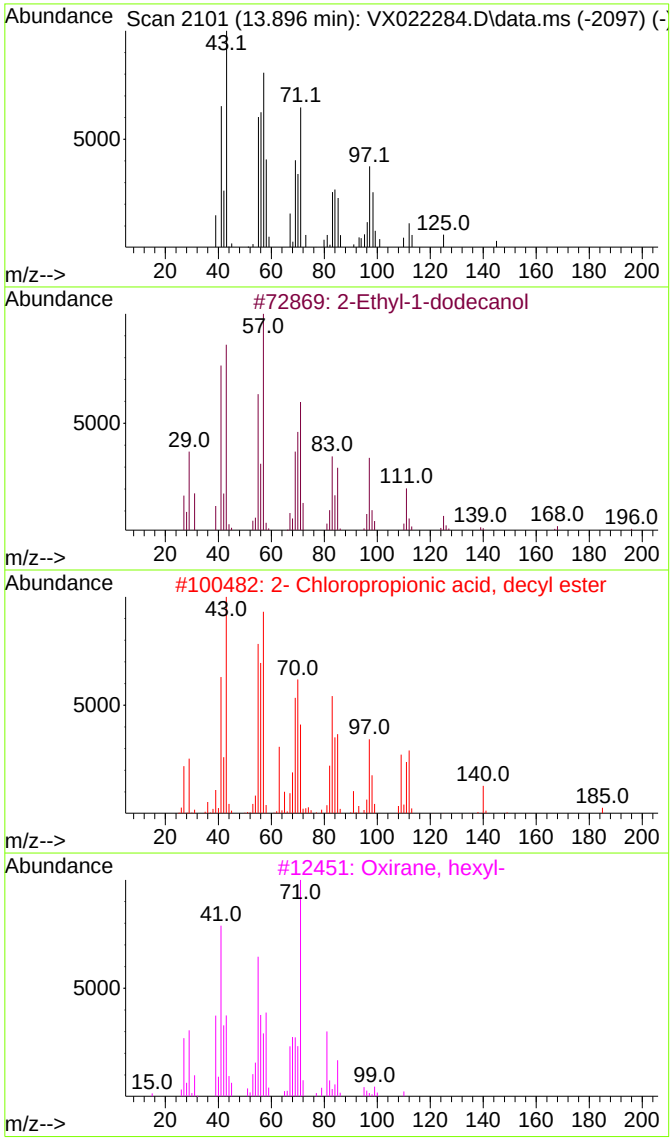
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

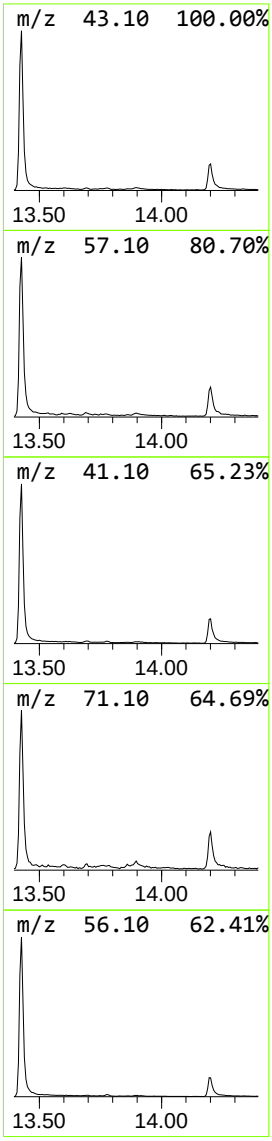
****

Peak Number 7 unknown13.896 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.896	6.45 ug/l	45618	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethyl-1-dodecanol	214	C14H30O	019780-33-7	49
2	2- Chloropropionic acid, decyl e...	248	C13H25ClO2	086711-78-6	43
3	Oxirane, hexyl-	128	C8H16O	002984-50-1	35
4	Formic acid, 2-methylpentyl ester	130	C7H14O2	381670-34-4	27
5	Oxalic acid, cyclobutyl octadecy...	396	C24H44O4	1000309-70-8	27





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TIC Library : C:\DATABASE\NIST11.L
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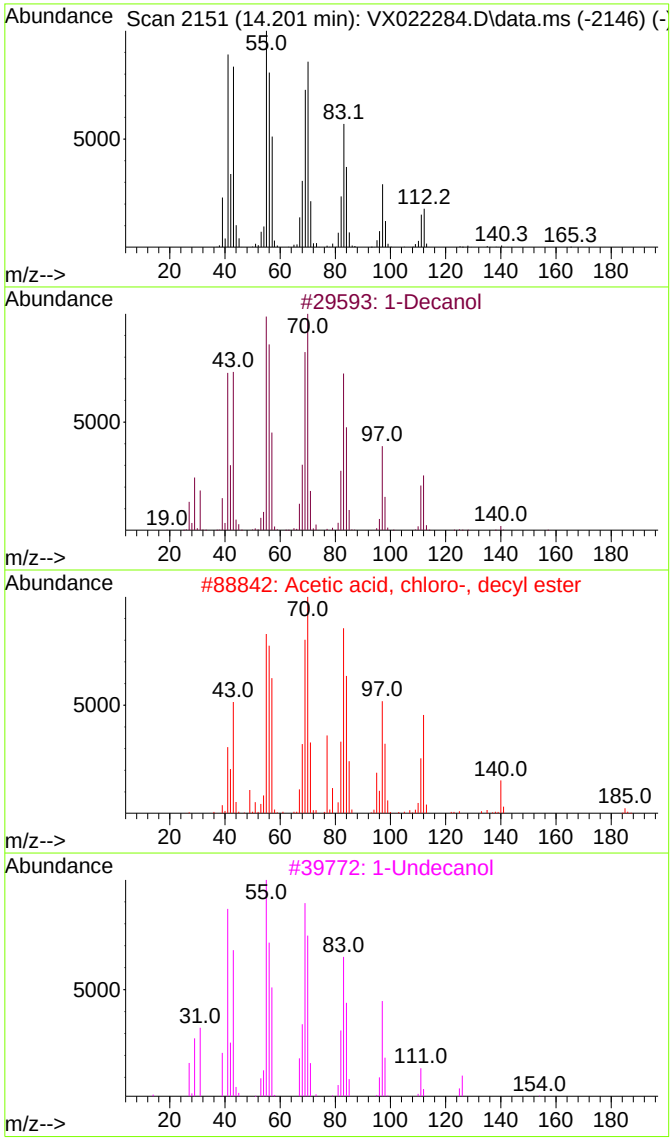
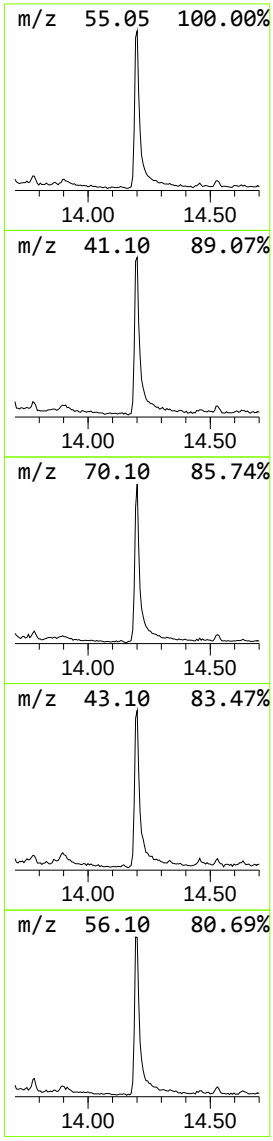
****
Peak Number 8 1-Decanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.201	87.39 ug/l	618464	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol	158	C10H22O	000112-30-1	90
2	Acetic acid, chloro-, decyl ester	234	C12H23ClO2	006974-05-6	90
3	1-Undecanol	172	C11H24O	000112-42-5	86
4	Formic acid, decyl ester	186	C11H22O2	005451-52-5	83
5	Cyclooctane	112	C8H16	000292-64-8	81





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Instrument :
MSVOA_X
ClientSampleId :
1917

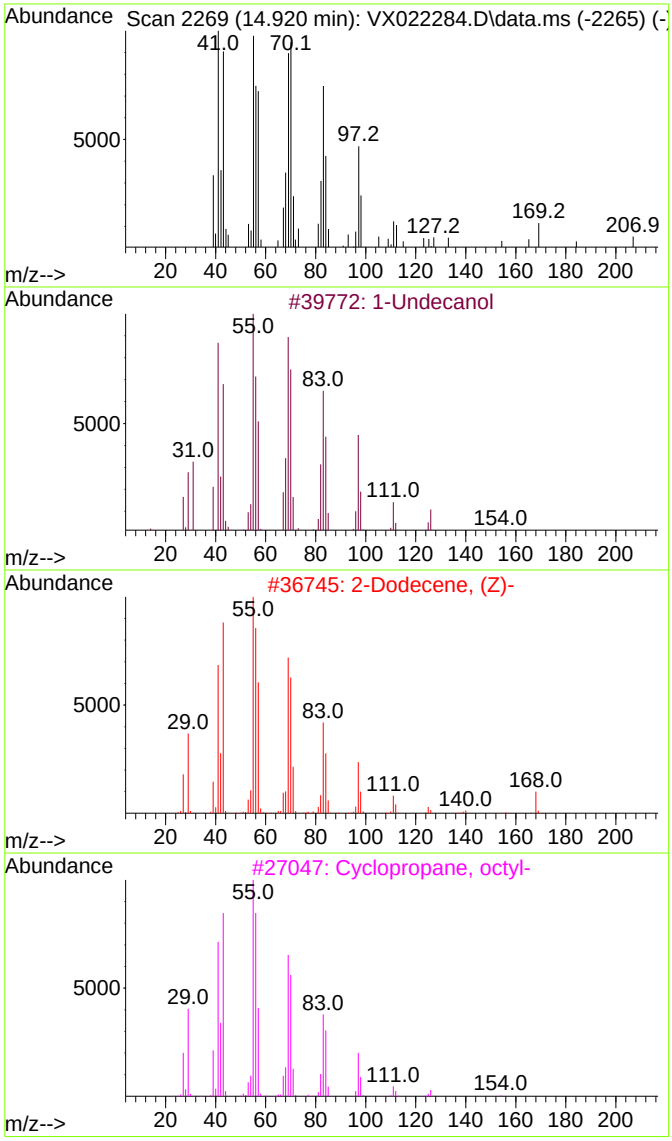
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

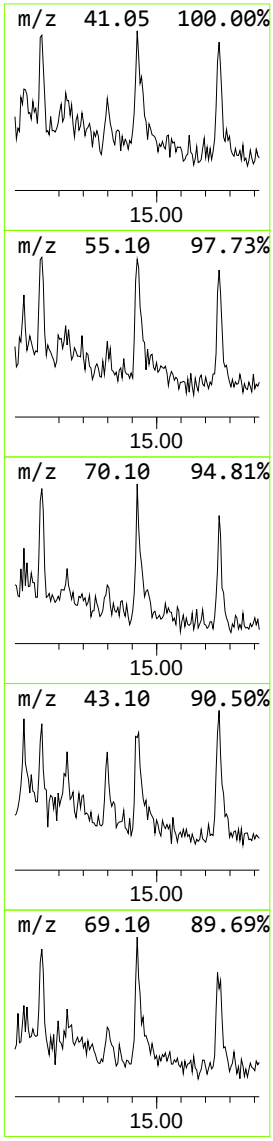
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1-Undecanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.920	5.53 ug/l	39109	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Undecanol	172	C11H24O	000112-42-5	91
2	2-Dodecene, (Z)-	168	C12H24	007206-26-0	90
3	Cyclopropane, octyl-	154	C11H22	001472-09-9	87
4	1-Decanol	158	C10H22O	000112-30-1	86
5	Carbonochloridic acid, decyl ester	220	C11H21ClO2	055488-51-2	86





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Acq On : 29 May 2021 04:38
Operator : JC/MD
Sample : M2517-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1917

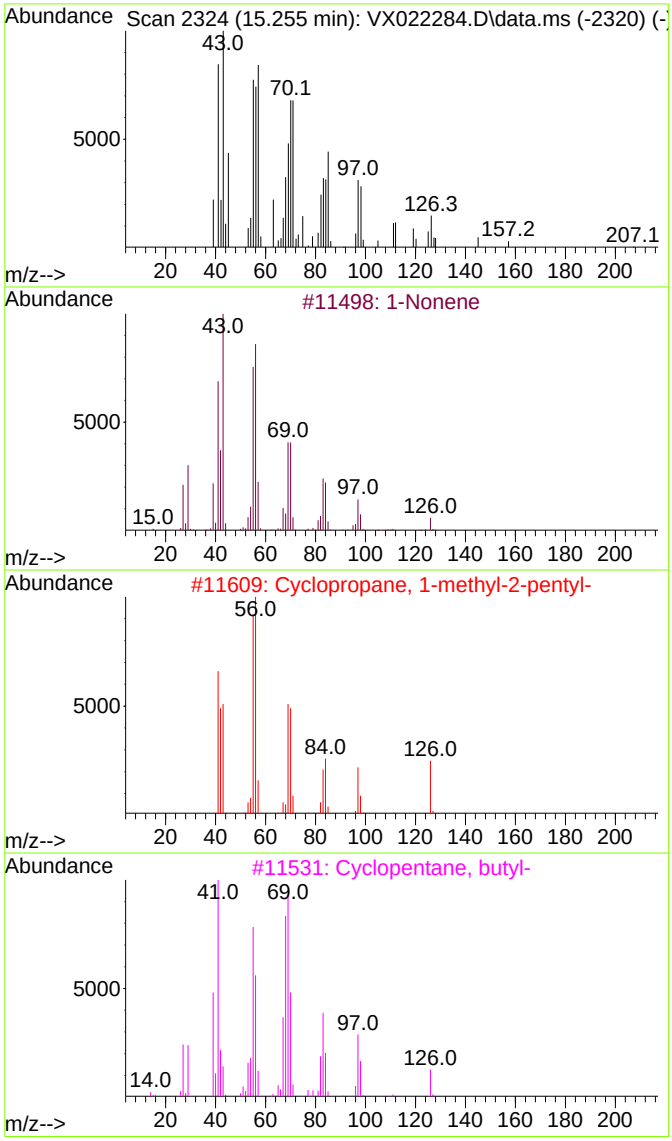
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

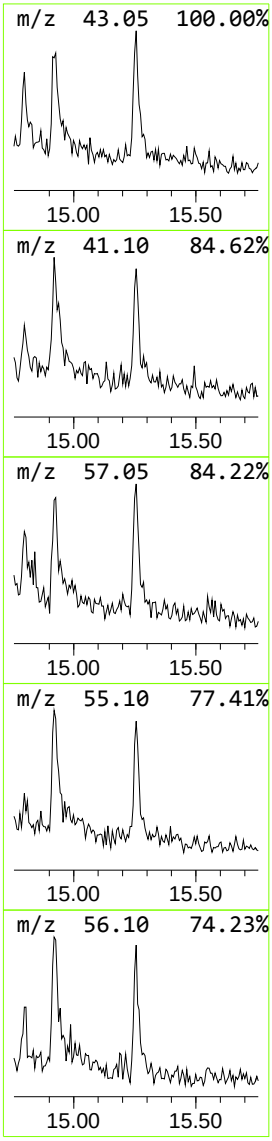
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 unknown15.255 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.255	5.01 ug/l	35435	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonene	126	C9H18	000124-11-8	50
2	Cyclopropane, 1-methyl-2-pentyl-	126	C9H18	041977-37-1	46
3	Cyclopentane, butyl-	126	C9H18	002040-95-1	46
4	1-Decene	140	C10H20	000872-05-9	46
5	Cycloheptane	98	C7H14	000291-64-5	41





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX052921\
Data File : VX022284.D
Acq On : 29 May 2021 04:38
Operator : JC/MD
Sample : M2517-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 40 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1917

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051921W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol	2.124	19.7	ug/l	84030	1	5.556	213187	50.0
1-Hexanol, 2-et...	12.219	156.7	ug/l	1108880	4	12.024	353833	50.0
Formic acid, oc...	12.591	7.9	ug/l	55672	4	12.024	353833	50.0
1-Nonene	13.103	5.0	ug/l	35580	4	12.024	353833	50.0
5-(Methylamino)...	13.140	5.1	ug/l	35972	4	12.024	353833	50.0
1-Nonanol	13.426	380.5	ug/l	2692940	4	12.024	353833	50.0
unknown13.896	13.896	6.5	ug/l	45618	4	12.024	353833	50.0
1-Decanol	14.201	87.4	ug/l	618464	4	12.024	353833	50.0
1-Undecanol	14.920	5.5	ug/l	39109	4	12.024	353833	50.0
unknown15.255	15.255	5.0	ug/l	35435	4	12.024	353833	50.0