LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112120\
Data File : VX019524.D
Acq On : 21 Nov 2020 03:57
Operator : JC/MD
Sample : L4779-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1608

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\82X112120W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.300	29	35	45	rBV	353218	1179547	2.16%	1.237%
2	5.623	732	744	762	rVB	330263	934232	1.71%	0.980%
3	6.830	931	942	961	rBV	525646	1499843	2.75%	1.573%
4	8.695	1241	1248	1254	rBV	1024751	1588385	2.91%	1.666%
5	10.098	1467	1478	1485	rBV	957715	1352246	2.48%	1.418%
6	11.122	1640	1646	1652	rBV	799364	1017268	1.87%	1.067%
7	12.061	1795	1800	1806	rVB	1036254	1262510	2.32%	1.324%
8	12.140	1806	1813	1823	rBV	1419475	1888682	3.47%	1.980%
9	13.134	1973	1976	1980	rBV	2357532	2876170	5.28%	3.016%
10	13.164	1980	1981	1991	rVB	644485	816589	1.50%	0.856%
11	13.469	2025	2031	2040	rBV	41595808	54506974	100.00%	57.154%
12	13.548	2040	2044	2052	rVB	665028	1001126	1.84%	1.050%
13	13.938	2104	2108	2118	rVB6	355162	857612	1.57%	0.899%
14	14.231	2152	2156	2168	rBV	9958273	11878548	21.79%	12.455%
15	14.652	2222	2225	2232	rBV3	524686	965998	1.77%	1.013%
16	14.890	2260	2264	2272	rVB3	575029	766547	1.41%	0.804%
17	15.469	2354	2359	2365	rVB	1869285	2755756	5.06%	2.890%
18	15.530	2365	2369	2371	rBV3	443591	698768	1.28%	0.733%
19	15.609	2379	2382	2387	rVB	869996	1291648	2.37%	1.354%
20	15.737	2399	2403	2407	rVV2	541601	835150	1.53%	0.876%
21	15.798	2408	2413	2419	rVB	1635446	2829811	5.19%	2.967%
22	15.920	2429	2433	2438	rVB	615775	1067733	1.96%	1.120%
23	16.042	2450	2453	2466	rVB6	520532	1497333	2.75%	1.570%

Sum of corrected areas: 95368476

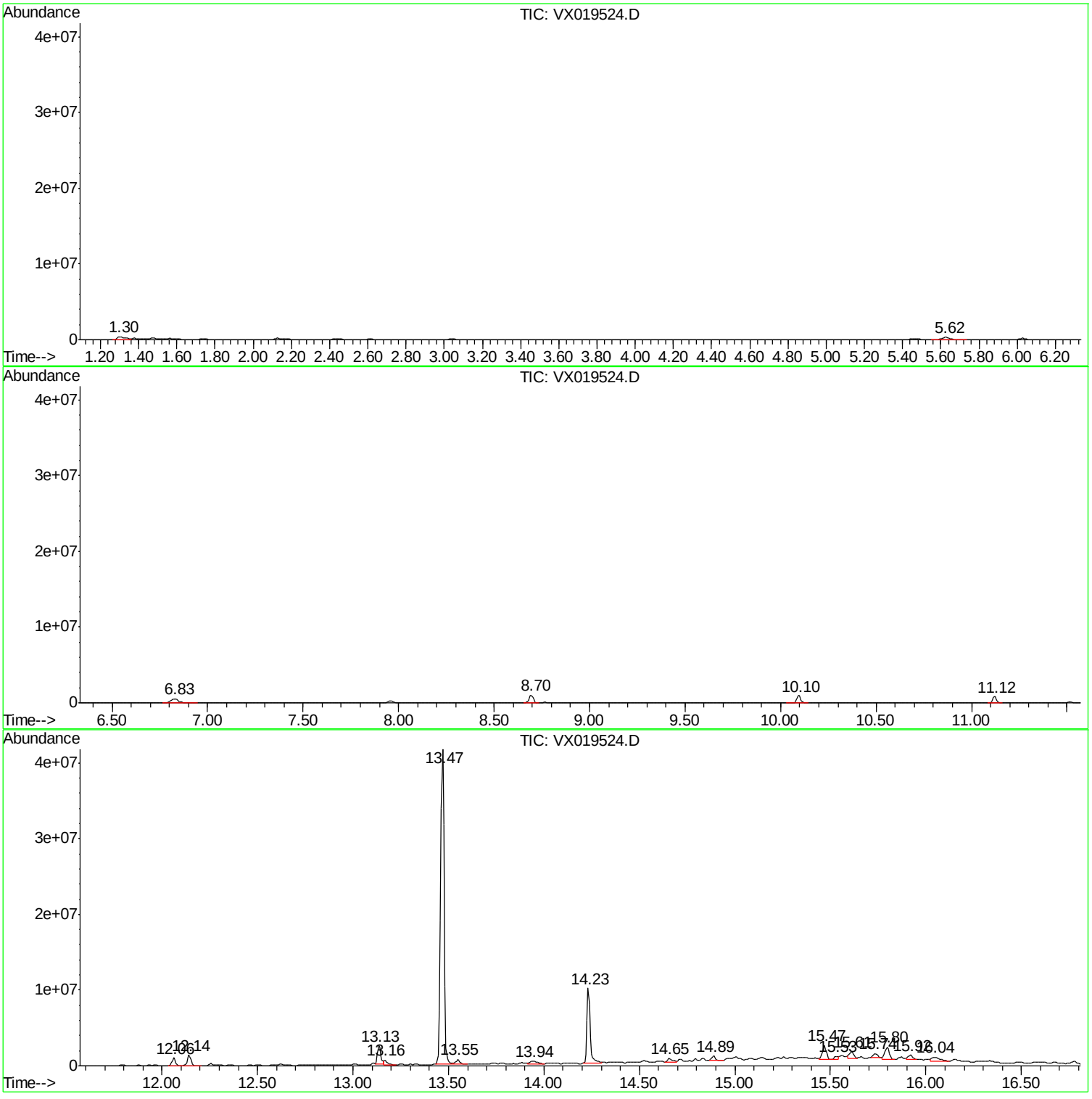
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112120\
Data File : VX019524.D
Acq On : 21 Nov 2020 03:57
Operator : JC/MD
Sample : L4779-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1608

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112120\
Data File : VX019524.D
Acq On : 21 Nov 2020 03:57
Operator : JC/MD
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Misc : 5.0mL/MSVOA X/WATER
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Quant Title : SW846 8260

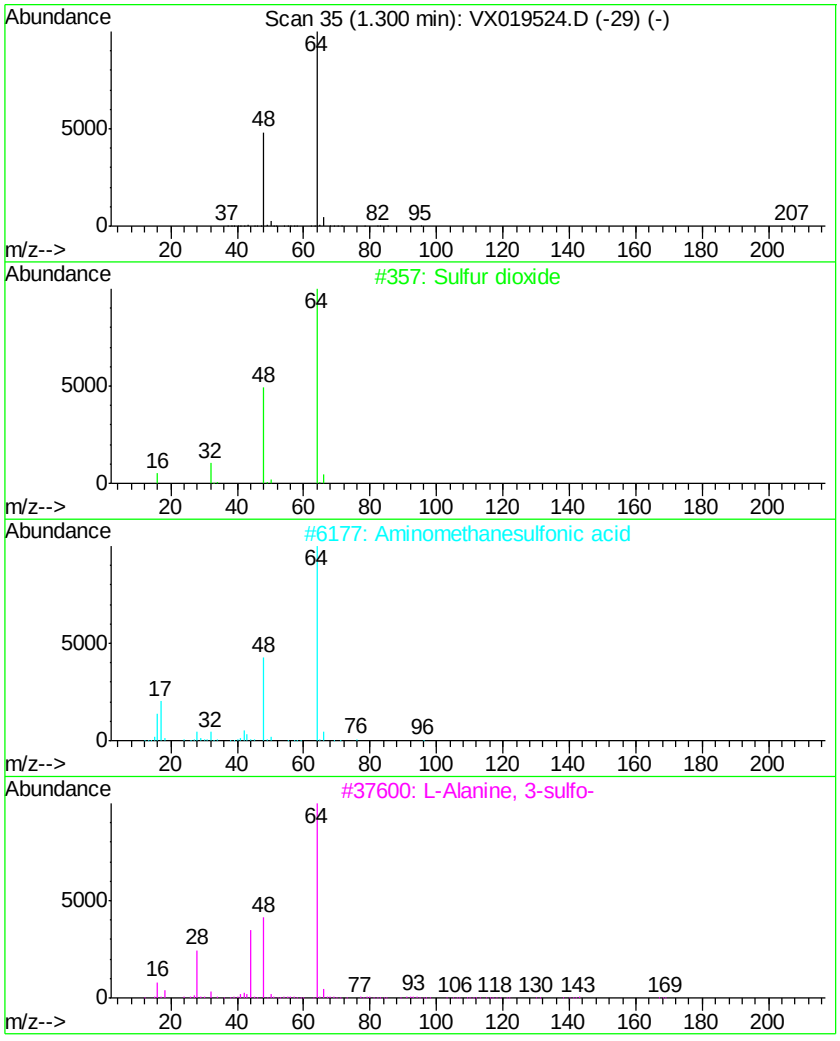
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

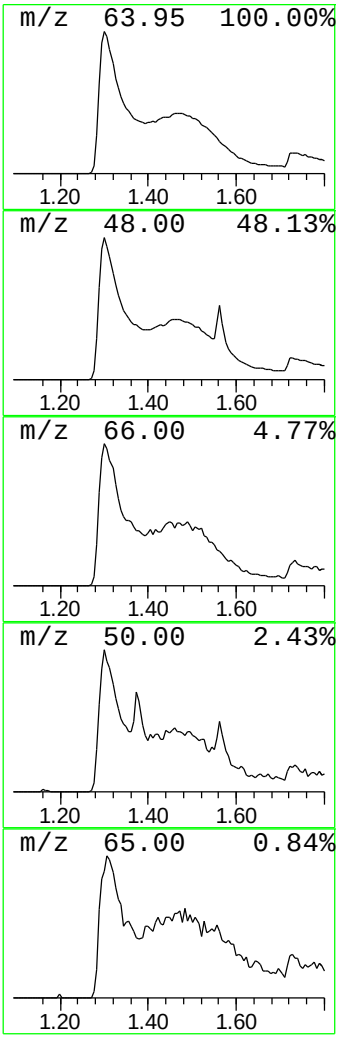
****

Peak Number 1 Sulfur dioxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.30	63.13 ug/l	1179550	Pentafluorobenzene	5.62

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	3





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112120\
Data File : VX019524.D
Acq On : 21 Nov 2020 03:57
Operator : JC/MD
Sample : L4779-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1608

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

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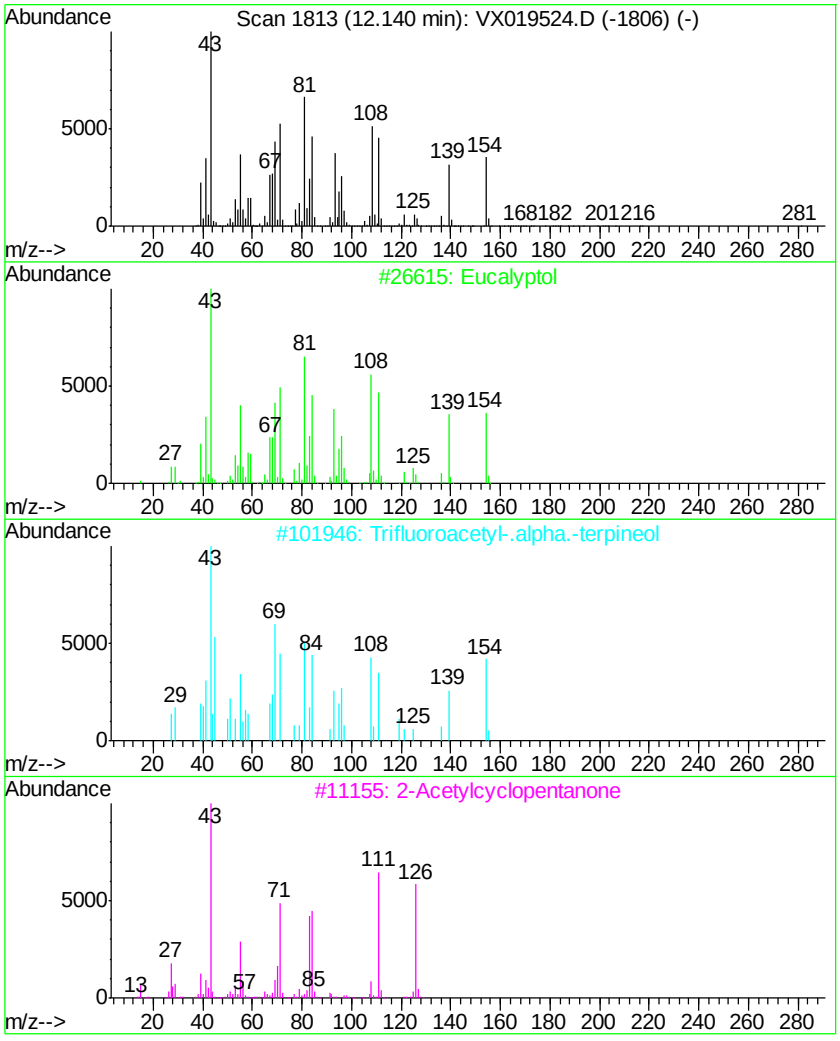
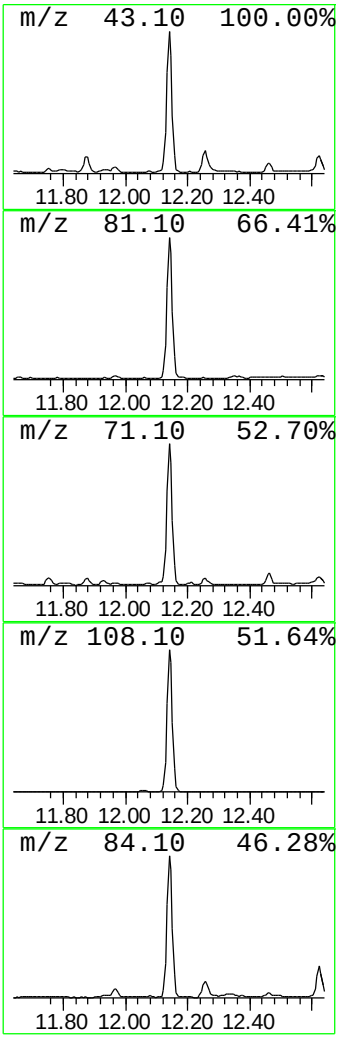
Peak Number 2 Eucalyptol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.14	74.80 ug/l	1888680	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	99
2	Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	47
3	2-Acetylcyclopentanone	126	C7H10O2	001670-46-8	35
4	3-Hepten-2-one, 3-propyl-	154	C10H18O	032064-69-0	25
5	5-Hepten-2-one, 6-methyl-	126	C8H14O	000110-93-0	25





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112120\
Data File : VX019524.D
Acq On : 21 Nov 2020 03:57
Operator : JC/MD
Sample : L4779-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1608

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

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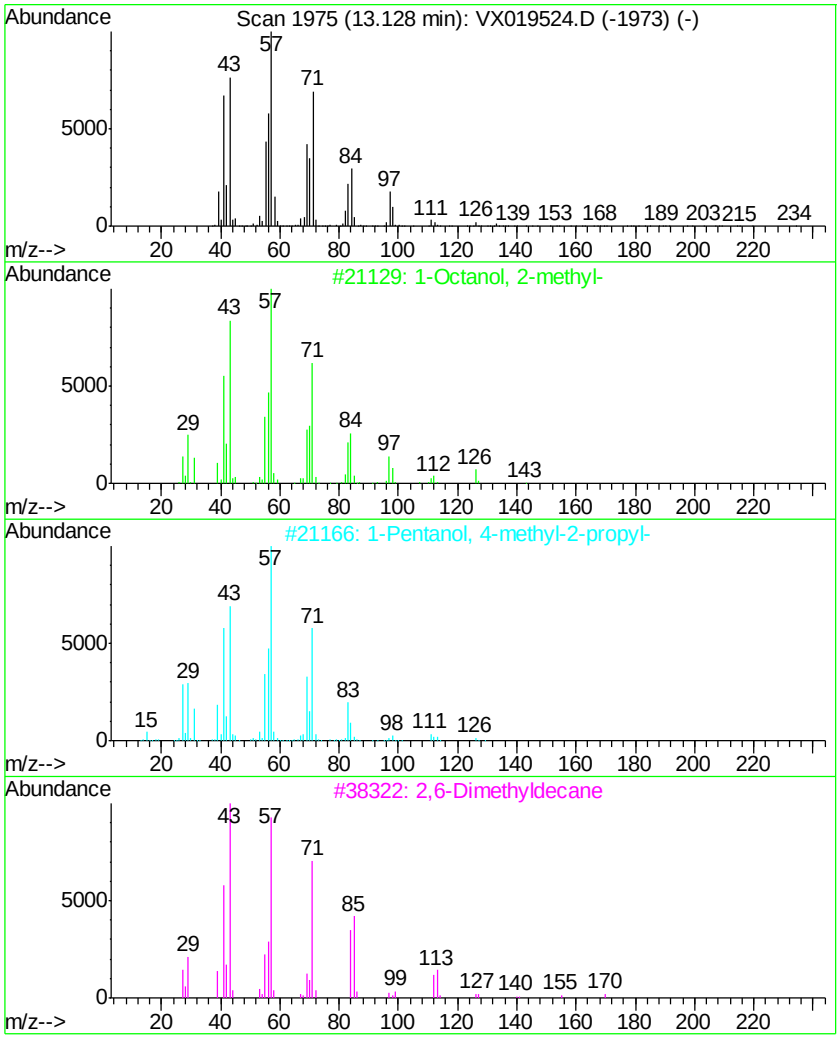
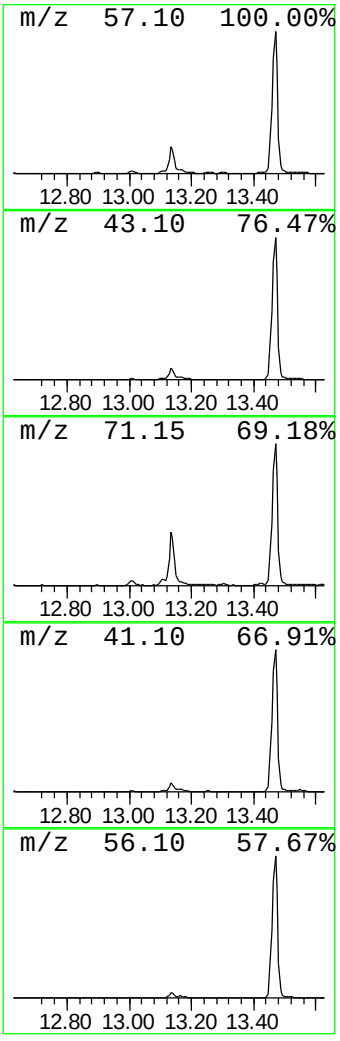
Peak Number 3 1-Octanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.13	113.91 ug/l	2876170	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	83
2	1-Pentanol, 4-methyl-2-propyl-	144	C9H20O	054004-41-0	59
3	2,6-Dimethyldecane	170	C12H26	013150-81-7	47
4	Isooctyl mercaptoacetate	204	C10H20O2S	025103-09-7	43
5	1-Dodecene	168	C12H24	000112-41-4	43





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112120\
Data File : VX019524.D
Acq On : 21 Nov 2020 03:57
Operator : JC/MD
Sample : L4779-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1608

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

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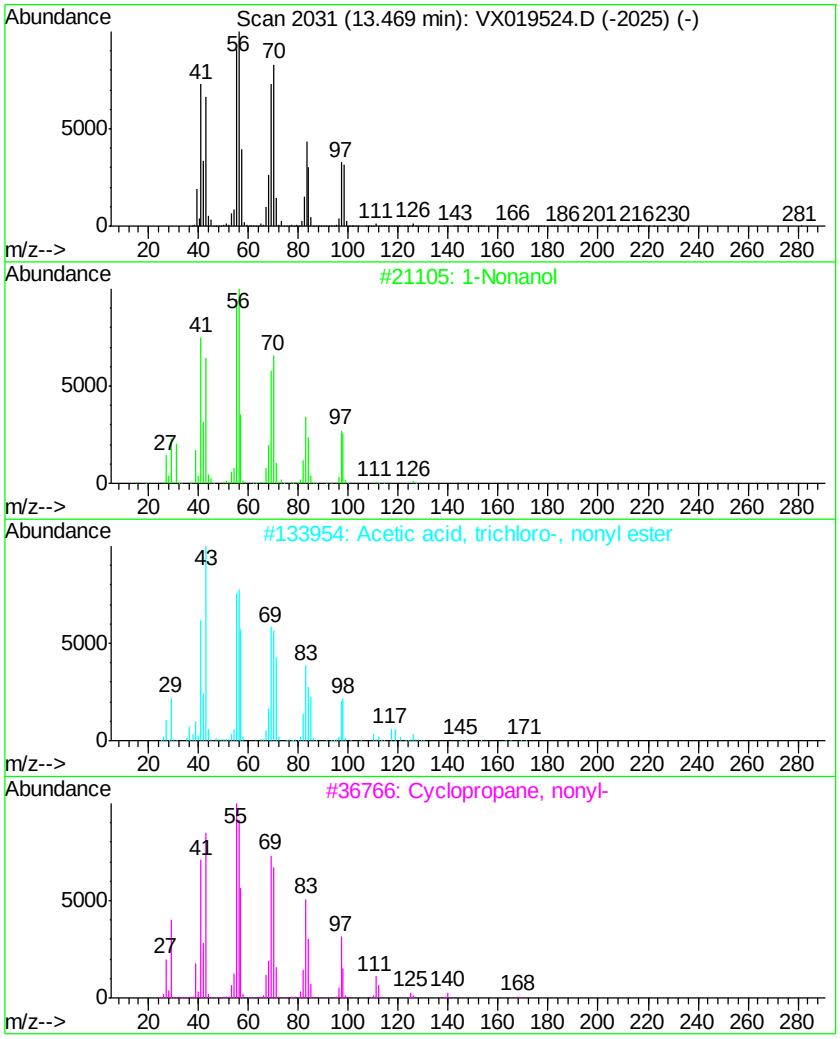
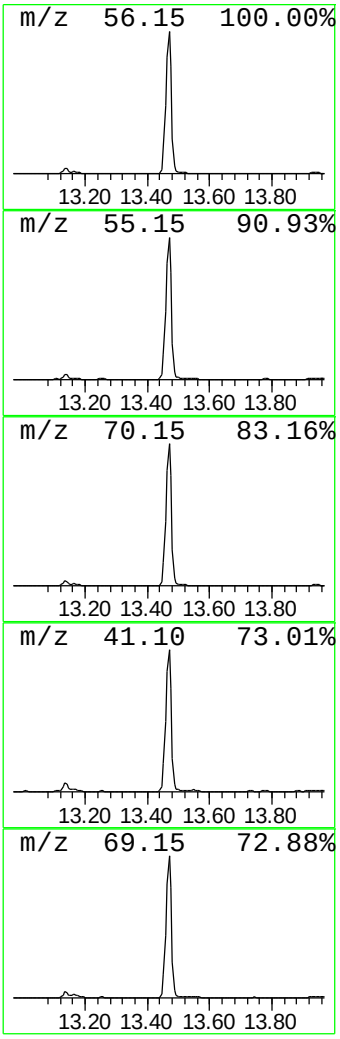
Peak Number 4 1-Nonanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	2158.67 ug/l	54507000	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonanol	144	C9H20O	000143-08-8	91
2	Acetic acid, trichloro-, nonyl e...	288	C11H19Cl3O2	065611-32-7	90
3	Cyclopropane, nonyl-	168	C12H24	074663-85-7	87
4	1-Dodecene	168	C12H24	000112-41-4	80
5	Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	78





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112120\
Data File : VX019524.D
Acq On : 21 Nov 2020 03:57
Operator : JC/MD
Sample : L4779-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1608

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

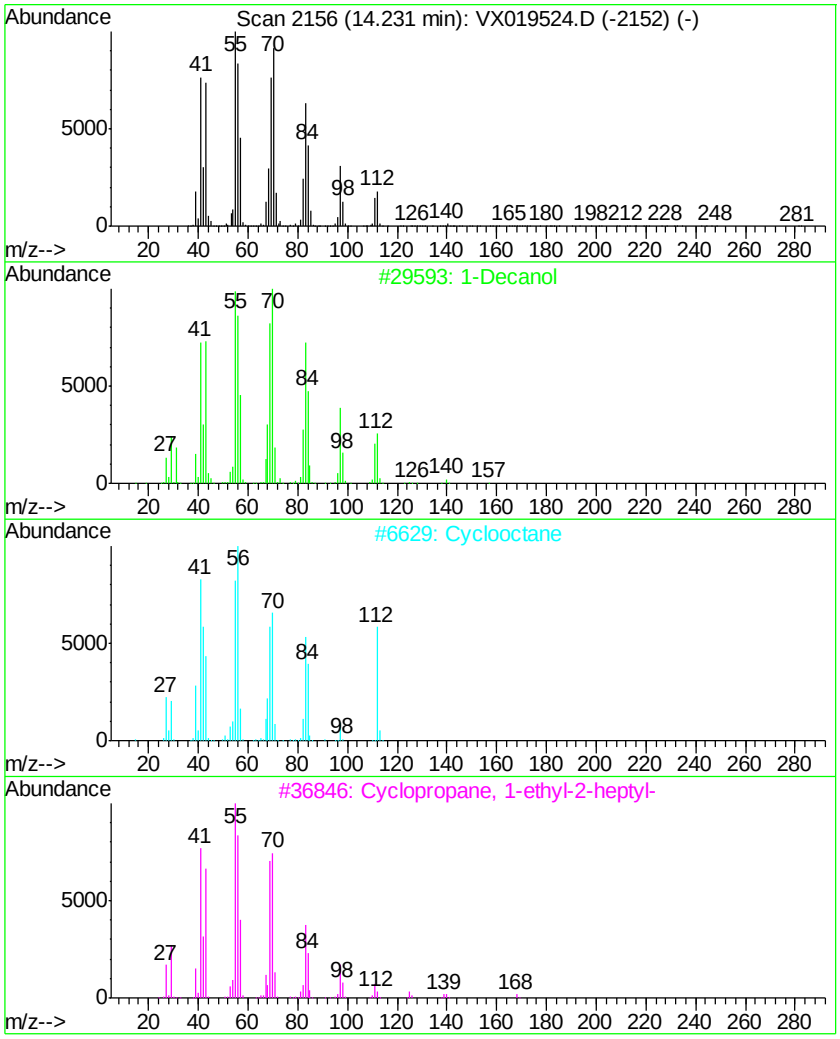
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

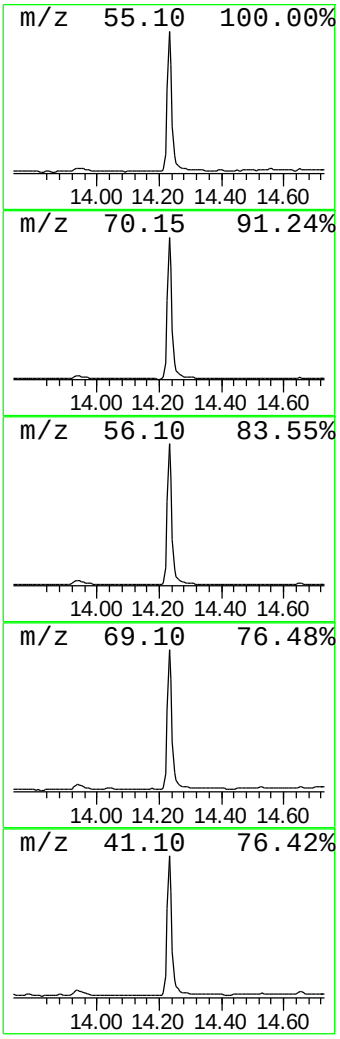
****

Peak Number 5 1-Decanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.23	470.43 ug/l	11878500	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol	158	C10H22O	000112-30-1	91
2	Cyclooctane	112	C8H16	000292-64-8	87
3	Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	86
4	1-Dodecene	168	C12H24	000112-41-4	86
5	Cyclopropane, 1-heptyl-2-methyl-	154	C11H22	074663-91-5	86





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112120\
Data File : VX019524.D
Acq On : 21 Nov 2020 03:57
Operator : JC/MD
Sample : L4779-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1608

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

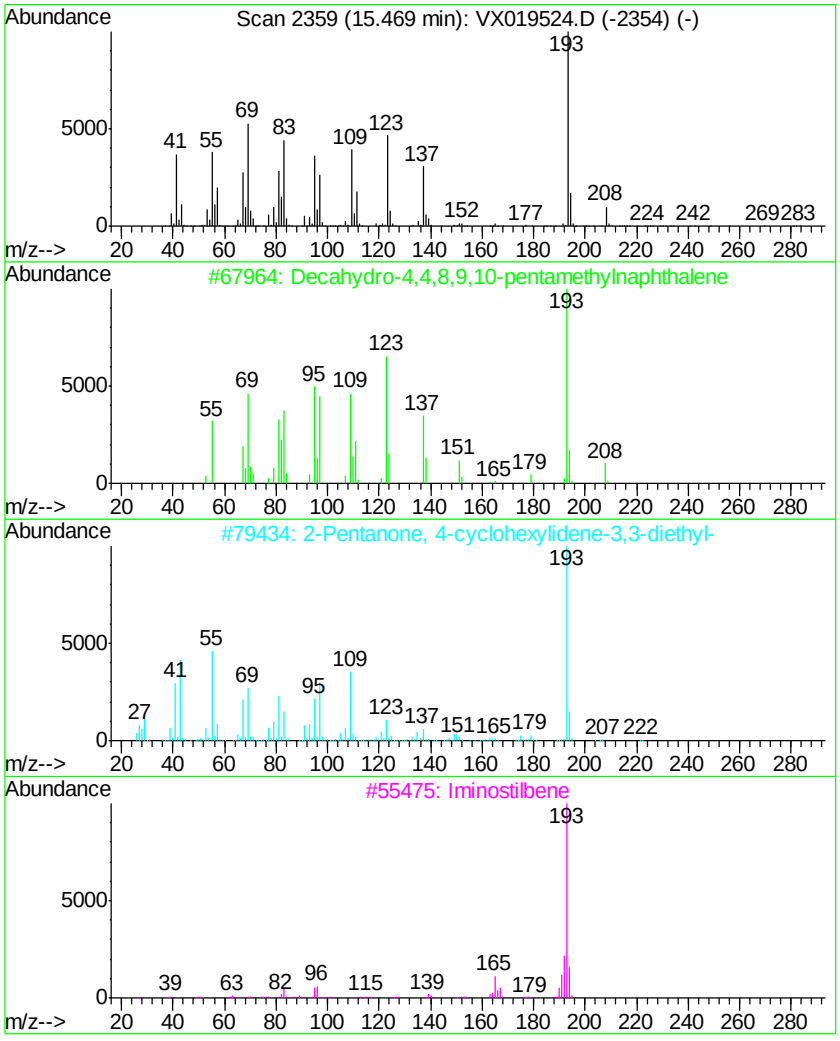
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

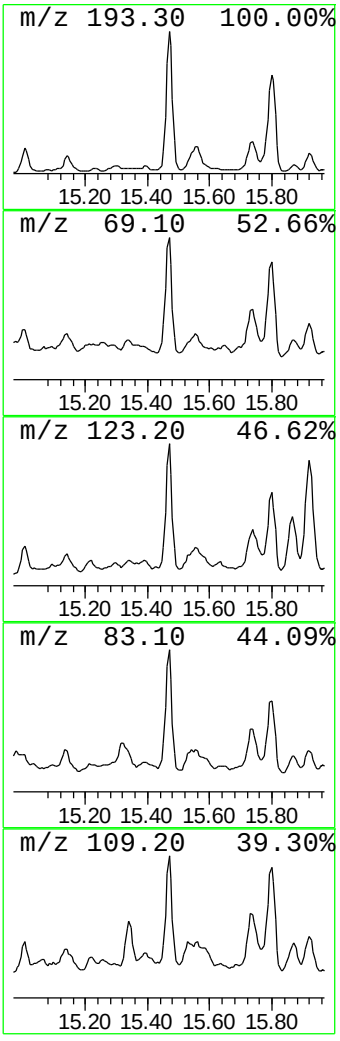
****

Peak Number 6 Decahydro-4,4,8,9,10-pentam... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.47	109.14 ug/l	2755760	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	74
2	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	47
3	Iminostilbene	193	C14H11N	000256-96-2	38
4	1H-Indene, octahydro-2,2,4,4,7,7...	208	C15H28	054832-83-6	37
5	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	32





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112120\
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ALS Vial : 43 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1608

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

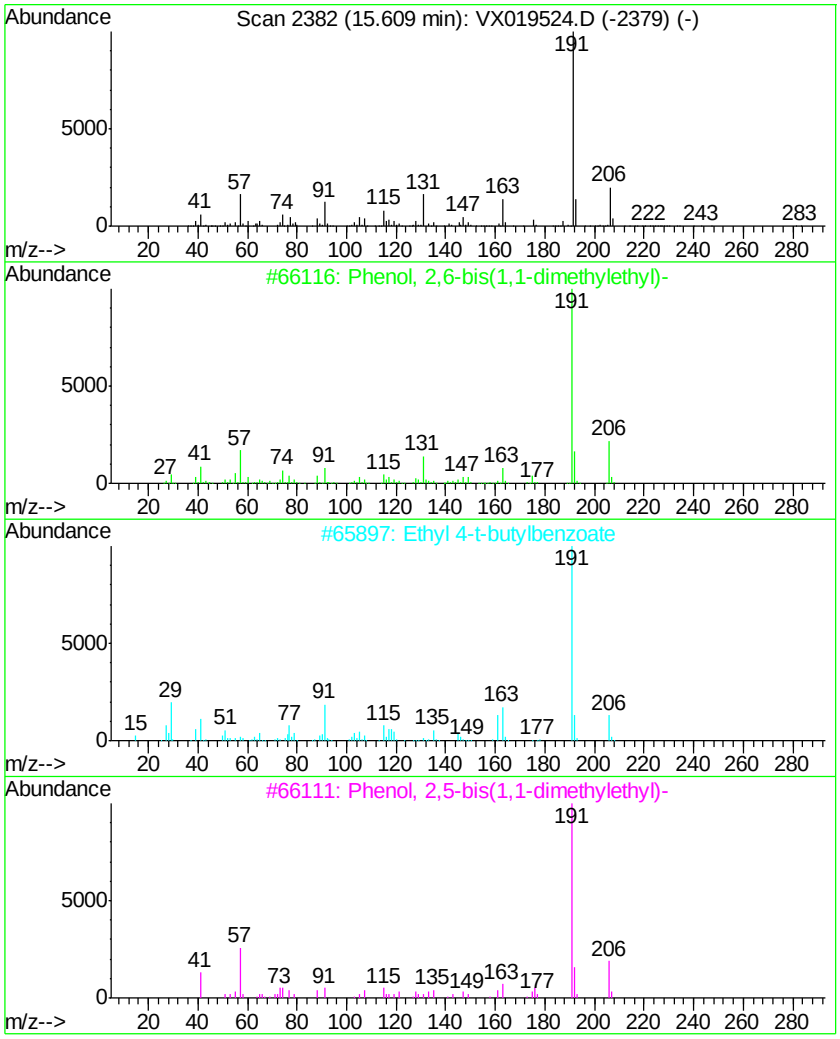
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

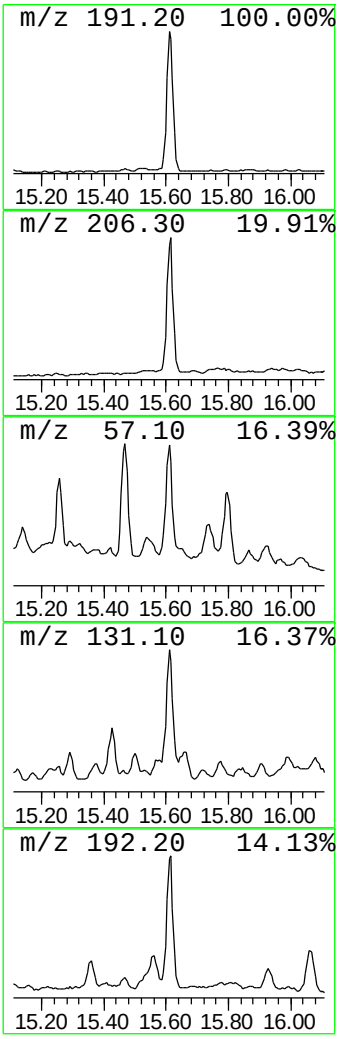
****

Peak Number 7 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.61	51.15 ug/l	1291650	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	93
2	Ethyl 4-t-butylbenzoate	206	C13H18O2	005406-57-5	87
3	Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	83
4	Phenol, 3,5-bis(1,1-dimethylethyl)-	206	C14H22O	001138-52-9	74
5	4'-Diethylaminoacetanilide	206	C12H18N2O	005326-57-8	72





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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1608

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

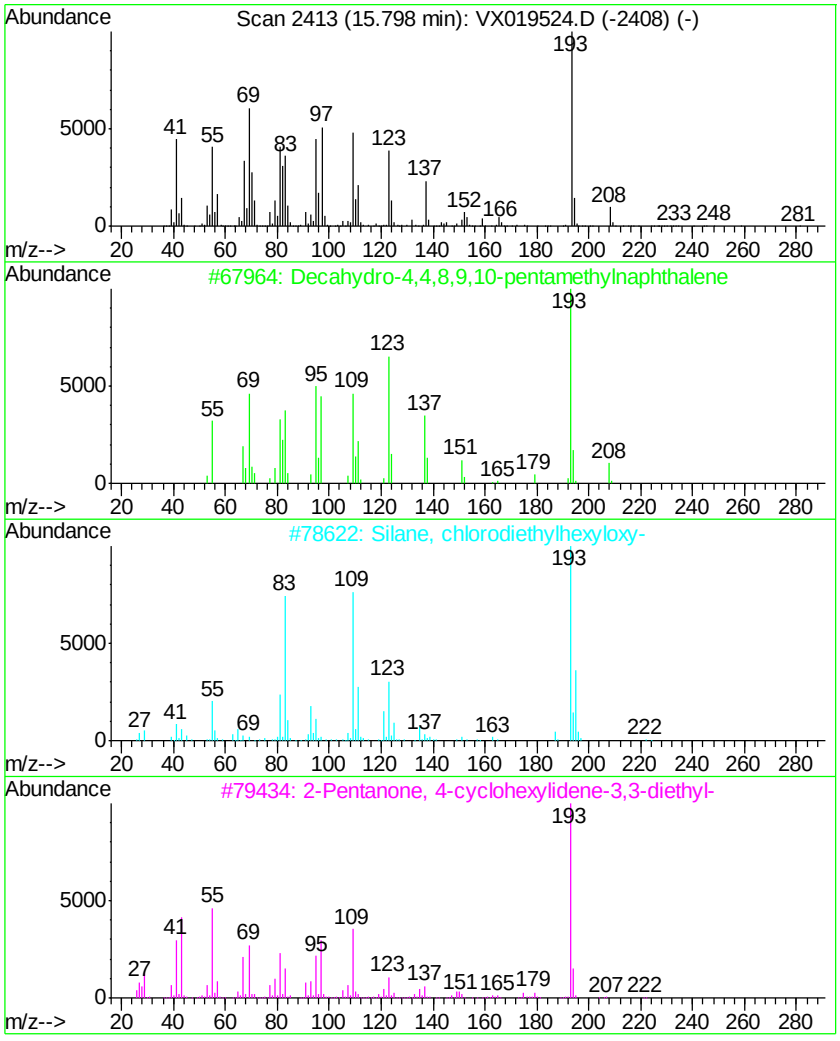
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

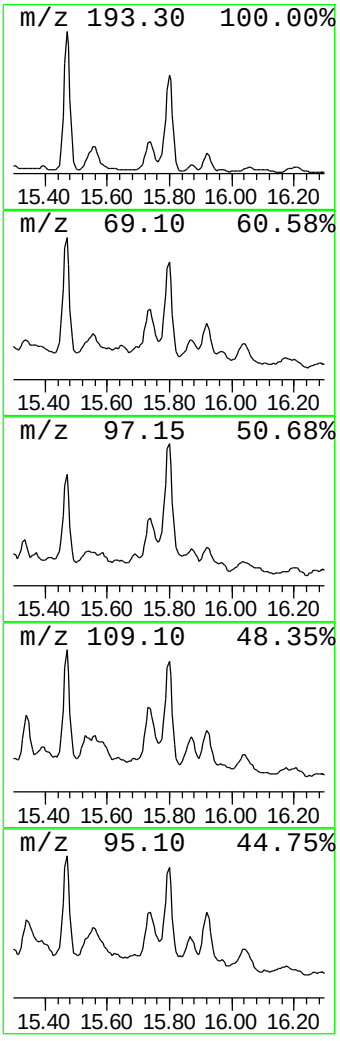
****

Peak Number 8 unknown15.80 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	112.07 ug/l	2829810	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decahydro-4,4,8,9,10-pentamethyl...	208	C15H28	080655-44-3	81
2	Silane, chlorodiethylhexyloxy-	222	C10H23ClOSi	1000363-74-4	43
3	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	38
4	1-(p-Fluorophenyl)-4-piperidone	193	C11H12FNO	1000238-56-7	35
5	Borinic acid, diethyl-, 3,3,5-tr...	208	C13H25BO	057387-76-5	32





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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1608

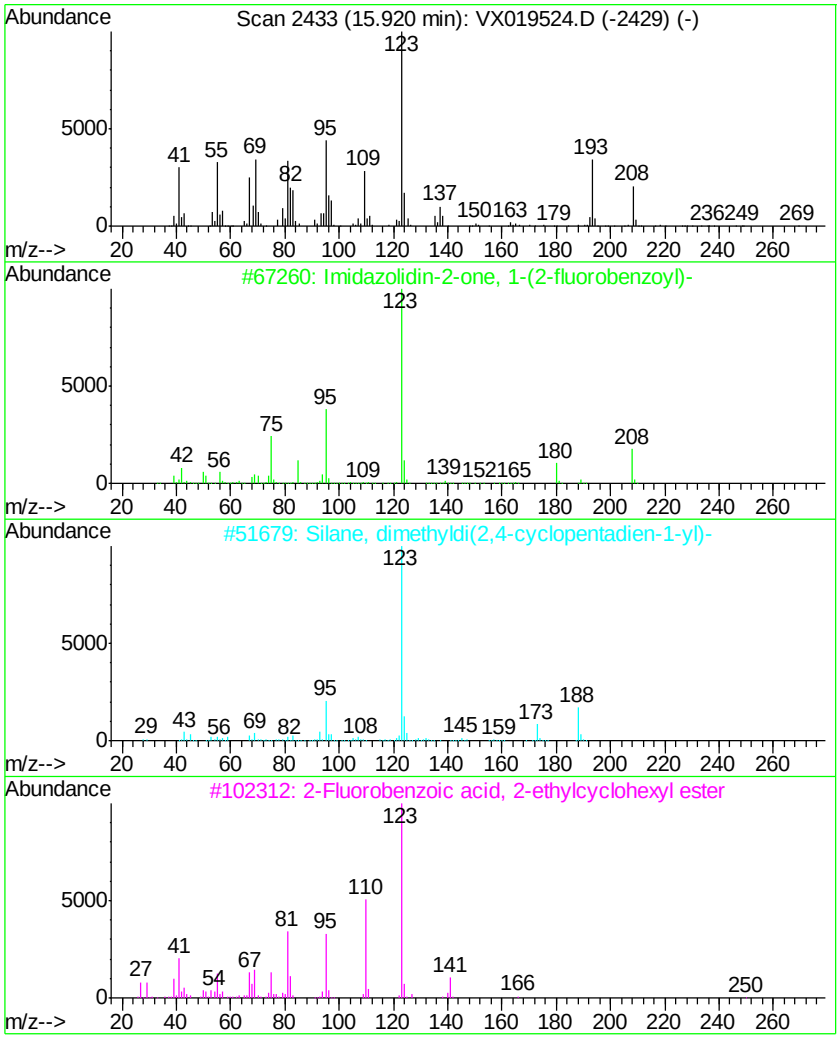
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

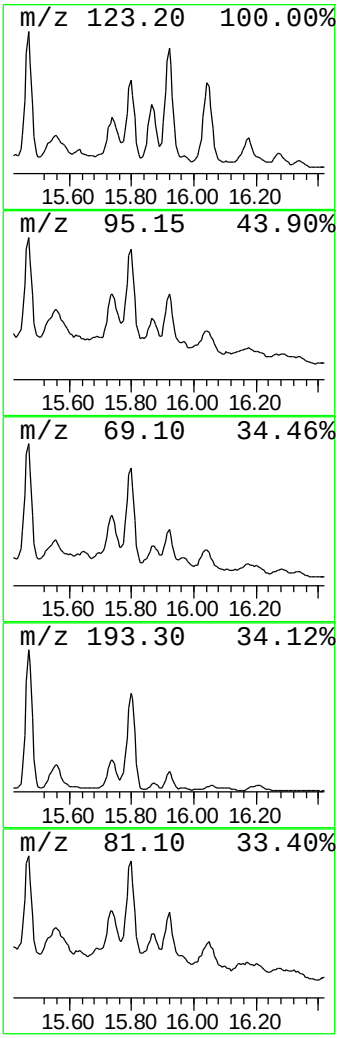
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Imidazolidin-2-one, 1-(2-fl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	42.29 ug/l	1067730	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Imidazolidin-2-one, 1-(2-fluorob...	208	C10H9FN2O2	1000310-62-2	52
2	Silane, dimethyldi(2,4-cyclopent...	188	C12H16Si	018053-74-2	47
3	2-Fluorobenzoic acid, 2-ethylcyc...	250	C15H19FO2	1000278-98-1	43
4	3-Fluorobenzoic acid, 1-cyclopen...	236	C14H17FO2	1000279-04-7	43
5	2-Fluorobenzoic acid, 1-cyclopen...	236	C14H17FO2	1000278-98-2	43





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112120\
Data File : VX019524.D
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ALS Vial : 43 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1608

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.M
Quant Title : SW846 8260

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

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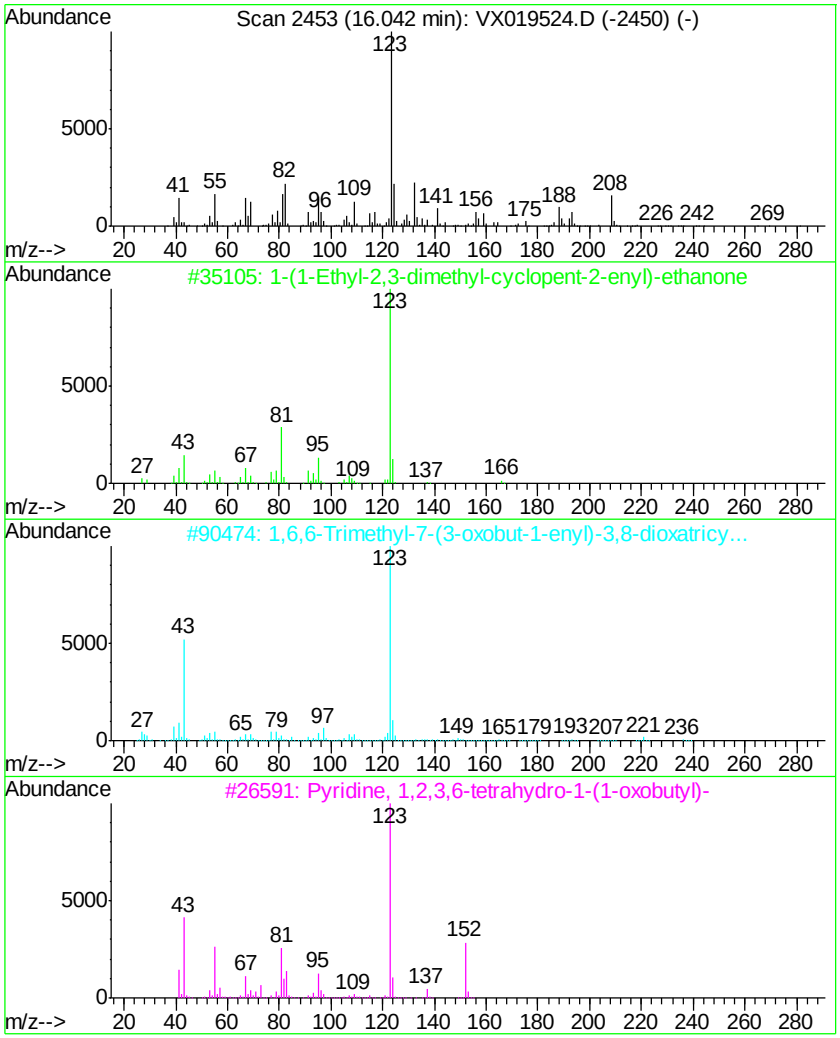
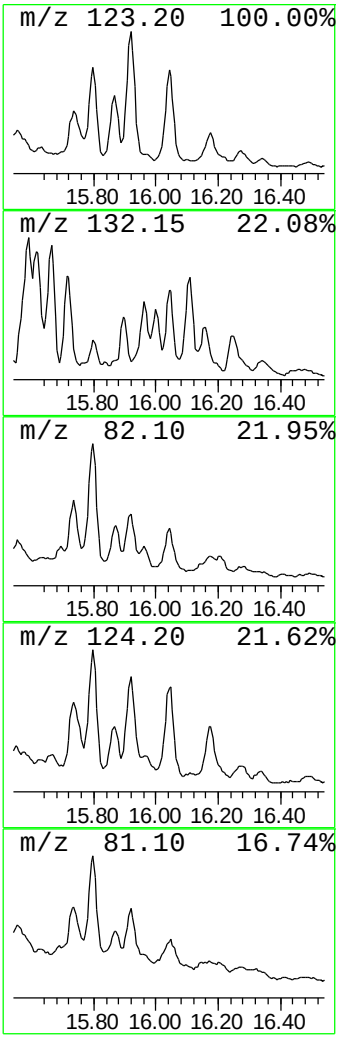
Peak Number 10 unknown16.04 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.04	59.30 ug/l	1497330	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(1-Ethyl-2,3-dimethyl-cyclopen...	166	C11H18O	1000185-18-6	43
2	1,6,6-Trimethyl-7-(3-oxobut-1-en...	236	C13H16O4	1000192-00-9	43
3	Pyridine, 1,2,3,6-tetrahydro-1-(...	153	C9H15NO	057150-46-6	43
4	2-Cyclopentene-1-carboxylic acid...	196	C12H20O2	1000195-65-9	38
5	2,6-Naphthalenedione, octahydro-...	208	C13H20O2	057289-17-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112120\
Data File : VX019524.D
Acq On : 21 Nov 2020 03:57
Operator : JC/MD
Sample : L4779-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1608

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112120W.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
Sulfur dioxide	1.30	63.1	ug/l	1179550	1	5.62	934232	50.0
Eucalyptol	12.14	74.8	ug/l	1888680	4	12.06	1262510	50.0
1-Octanol, 2-methyl-	13.13	113.9	ug/l	2876170	4	12.06	1262510	50.0
1-Nonanol	13.47	2158.7	ug/l	54507000	4	12.06	1262510	50.0
1-Decanol	14.23	470.4	ug/l	11878500	4	12.06	1262510	50.0
Decahydro-4,4,8,9...	15.47	109.1	ug/l	2755760	4	12.06	1262510	50.0
Phenol, 2,6-bis(1...	15.61	51.1	ug/l	1291650	4	12.06	1262510	50.0
unknown15.80	15.80	112.1	ug/l	2829810	4	12.06	1262510	50.0
Imidazolidin-2-on...	15.92	42.3	ug/l	1067730	4	12.06	1262510	50.0
unknown16.04	16.04	59.3	ug/l	1497330	4	12.06	1262510	50.0