LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112120\
Data File : VX019519.D
Acq On : 21 Nov 2020 02:00
Operator : JC/MD
Sample : L4779-02 10X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1641

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	1.471	59	63	71	rBV	162903	206983	2.77%	0.991%
2	2.178	171	179	191	rBV	572594	997078	13.35%	4.775%
3	2.331	199	204	213	rBV	139461	240217	3.22%	1.150%
4	2.434	213	221	233	rVB3	43237	130262	1.74%	0.624%
5	4.001	460	478	507	rBV	823748	2633146	35.25%	12.610%
6	5.172	657	670	682	rVB	28218	84471	1.13%	0.405%
7	5.464	705	718	732	rBV	144262	416402	5.58%	1.994%
8	5.623	732	744	761	rVV	269705	756595	10.13%	3.623%
9	6.031	799	811	828	rBV	167260	439373	5.88%	2.104%
10	6.830	930	942	962	rBV	406487	985124	13.19%	4.718%
11	8.695	1241	1248	1257	rBV	813954	1281974	17.16%	6.139%
12	10.097	1472	1478	1490	rBV	787473	1078321	14.44%	5.164%
13	10.981	1618	1623	1631	rBV	146763	204510	2.74%	0.979%
14	11.122	1640	1646	1653	rBV	665131	838532	11.23%	4.016%
15	11.463	1696	1702	1708	rBV	79319	103009	1.38%	0.493%
16	12.061	1795	1800	1808	rVB	811549	1020237	13.66%	4.886%
17	12.256	1827	1832	1846	rBV	6424585	7469015	100.00%	35.768%
18	13.457	2023	2029	2033	rBV5	34412	80055	1.07%	0.383%
19	14.670	2223	2228	2232	rBV5	46163	93495	1.25%	0.448%
20	14.713	2232	2235	2238	rBV3	61021	75111	1.01%	0.360%
21	15.225	2314	2319	2327	rBV5	98766	219950	2.94%	1.053%
22	15.426	2348	2352	2355	rBV3	76665	104326	1.40%	0.500%
23	15.462	2355	2358	2362	rVB2	75047	101180	1.35%	0.485%
24	15.529	2365	2369	2375	rVV2	78089	133285	1.78%	0.638%
25	15.584	2376	2378	2385	rVB3	55139	87074	1.17%	0.417%
26	15.664	2387	2391	2394	rBV	94605	134160	1.80%	0.642%
27	15.792	2406	2412	2417	rBV2	132687	274005	3.67%	1.312%
28	16.029	2446	2451	2460	rBV8	89640	221545	2.97%	1.061%
29	16.145	2466	2470	2475	rBV2	77701	140971	1.89%	0.675%
30	16.334	2496	2501	2502	rBV2	73442	119550	1.60%	0.573%
31	16.663	2551	2555	2560	rBV3	65873	124482	1.67%	0.596%
32	16.767	2568	2572	2575	rBV4	48947	87180	1.17%	0.417%

LSC Area Percent Report

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ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1641

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

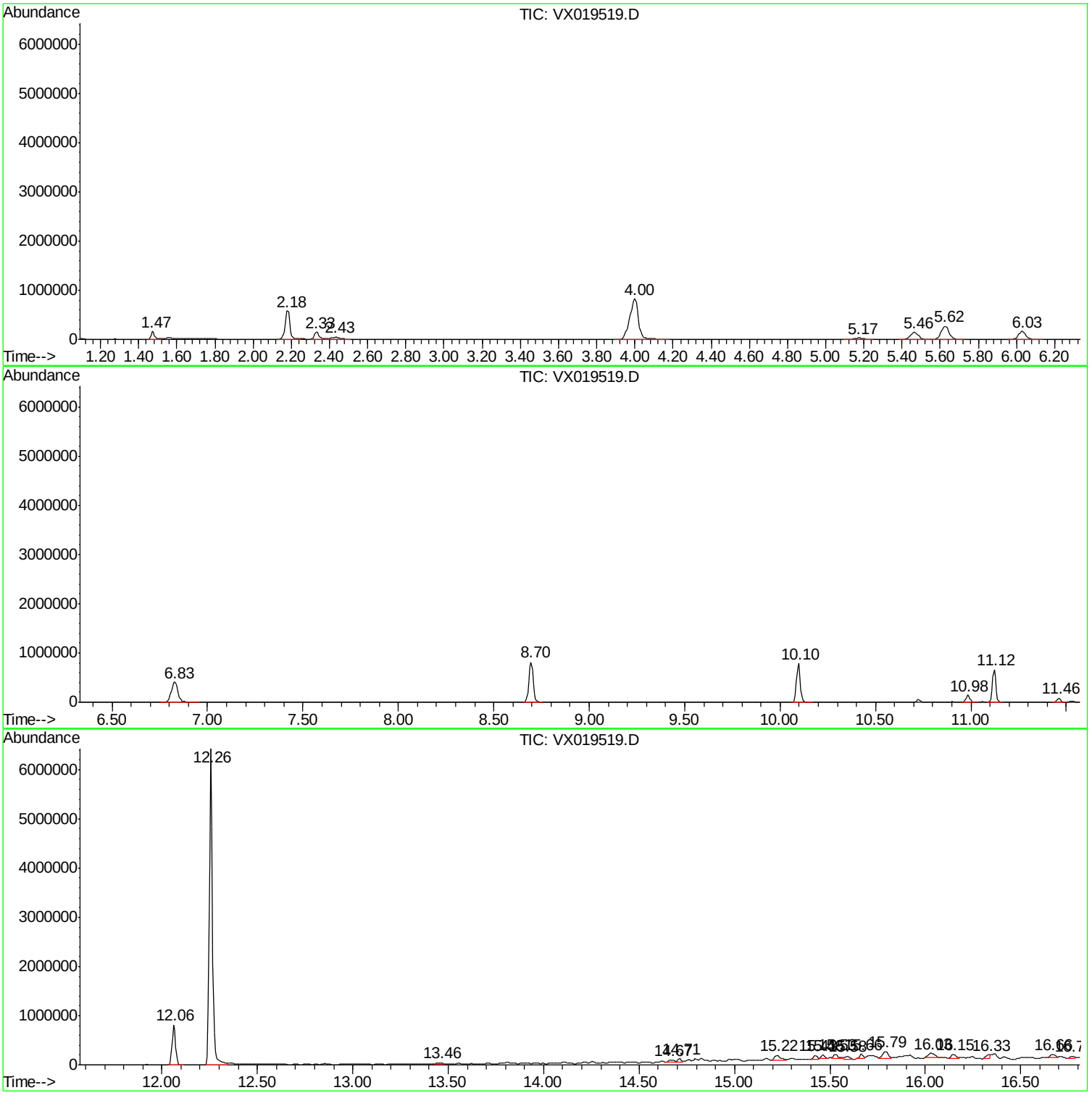
Sum of corrected areas: 20881618

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112120\
Data File : VX019519.D
Acq On : 21 Nov 2020 02:00
Operator : JC/MD
Sample : L4779-02 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1641

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

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Data File : VX019519.D
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Quant Title : SW846 8260

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

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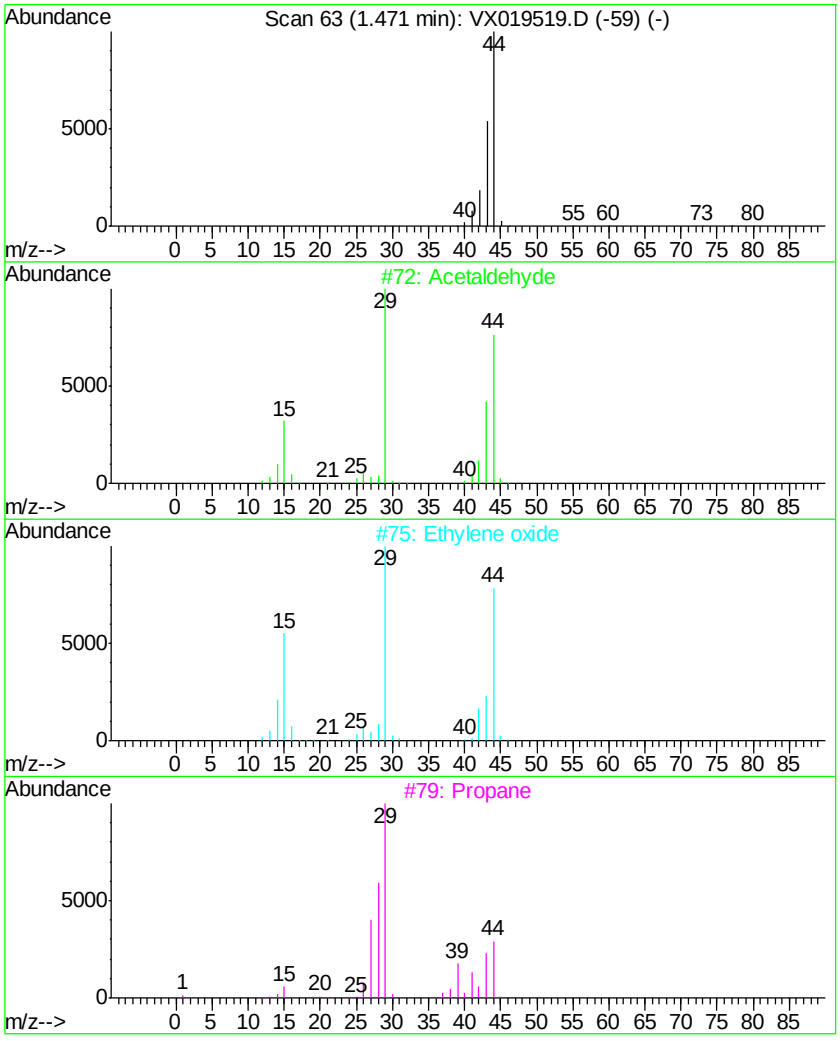
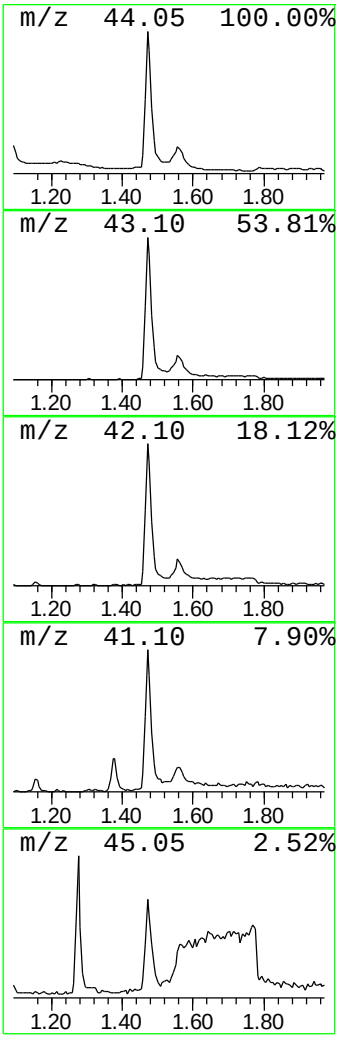
Peak Number 1 Acetaldehyde Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.47	13.68 ug/l	206983	Pentafluorobenzene	5.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	64
2	Ethylene oxide	44	C2H4O	000075-21-8	5
3	Propane	44	C3H8	000074-98-6	4
4	Alanine	89	C3H7NO2	000056-41-7	4
5	Ethyne, fluoro-	44	C2HF	002713-09-9	3





Library Search Compound Report

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Data File : VX019519.D
Acq On : 21 Nov 2020 02:00
Operator : JC/MD
Sample : L4779-02 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1641

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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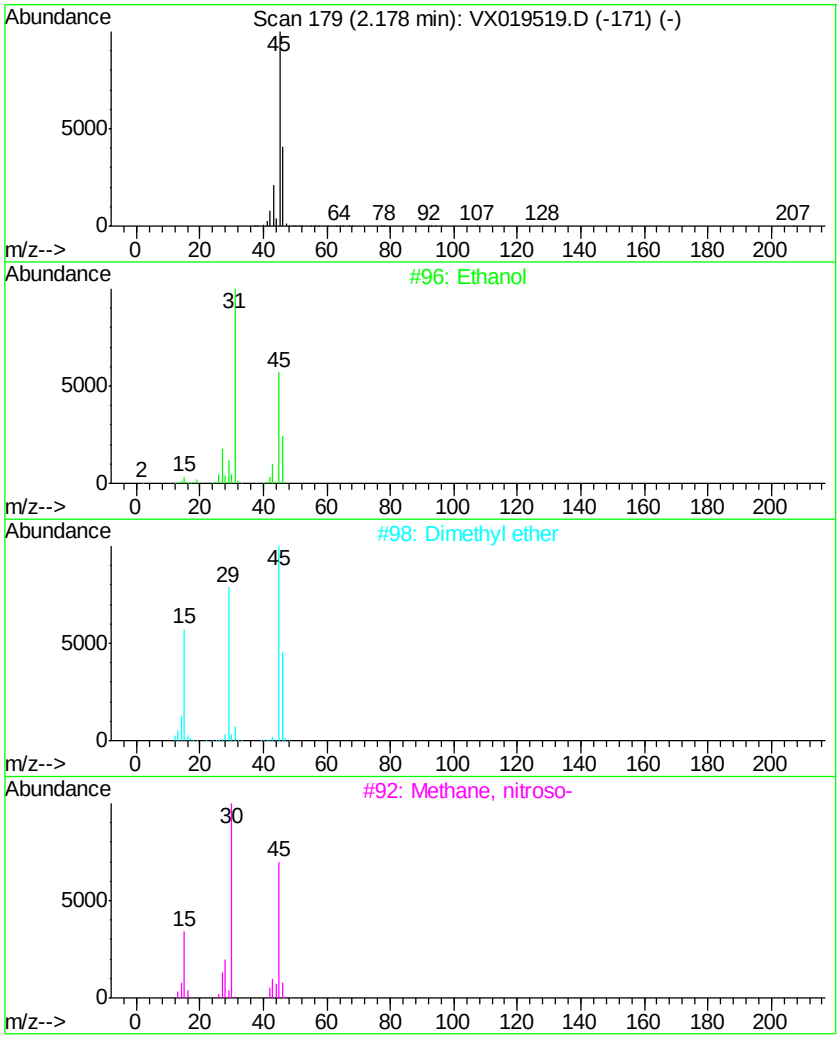
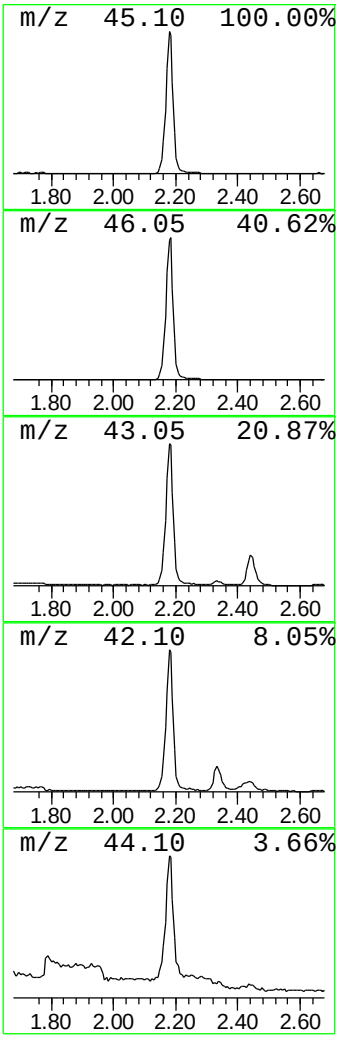
Peak Number 2 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	65.89 ug/l	997078	Pentafluorobenzene	5.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	64
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	Oxalic acid	90	C2H2O4	000144-62-7	4





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Data File : VX019519.D
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Operator : JC/MD
Sample : L4779-02 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1641

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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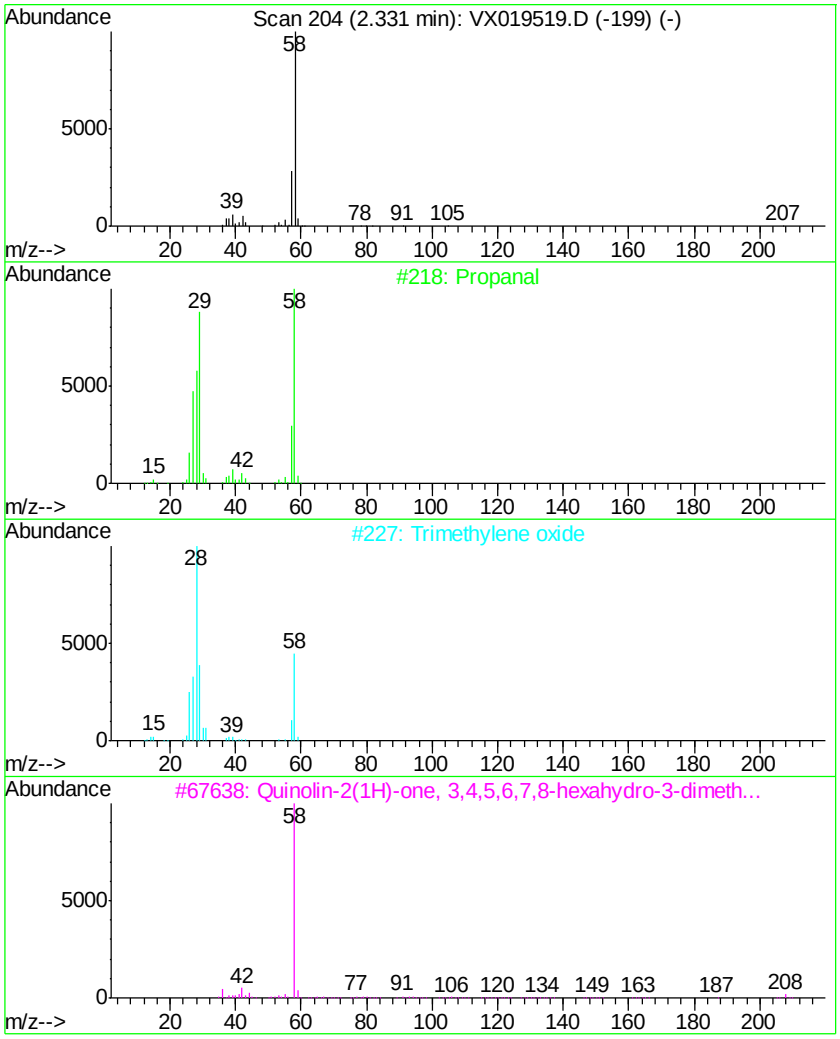
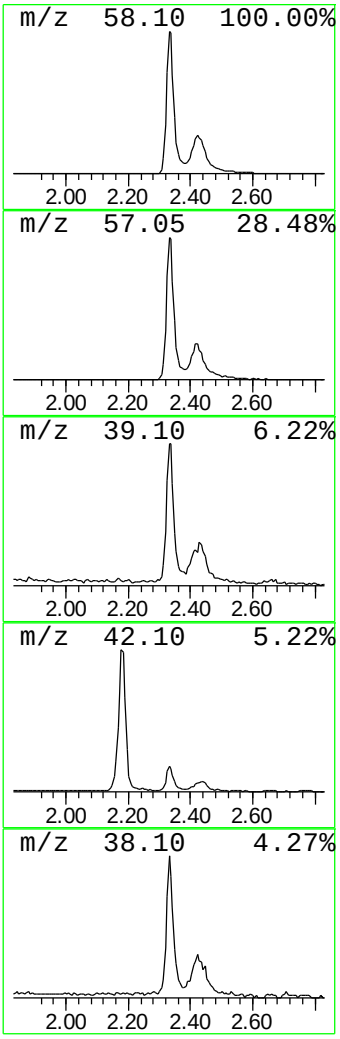
Peak Number 3 Propanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.33	15.87 ug/l	240217	Pentafluorobenzene	5.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	78
2	Trimethylene oxide	58	C3H6O	000503-30-0	56
3	Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
4	.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
5	Propylene oxide	58	C3H6O	000075-56-9	7





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112120\
Data File : VX019519.D
Acq On : 21 Nov 2020 02:00
Operator : JC/MD
Sample : L4779-02 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1641

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

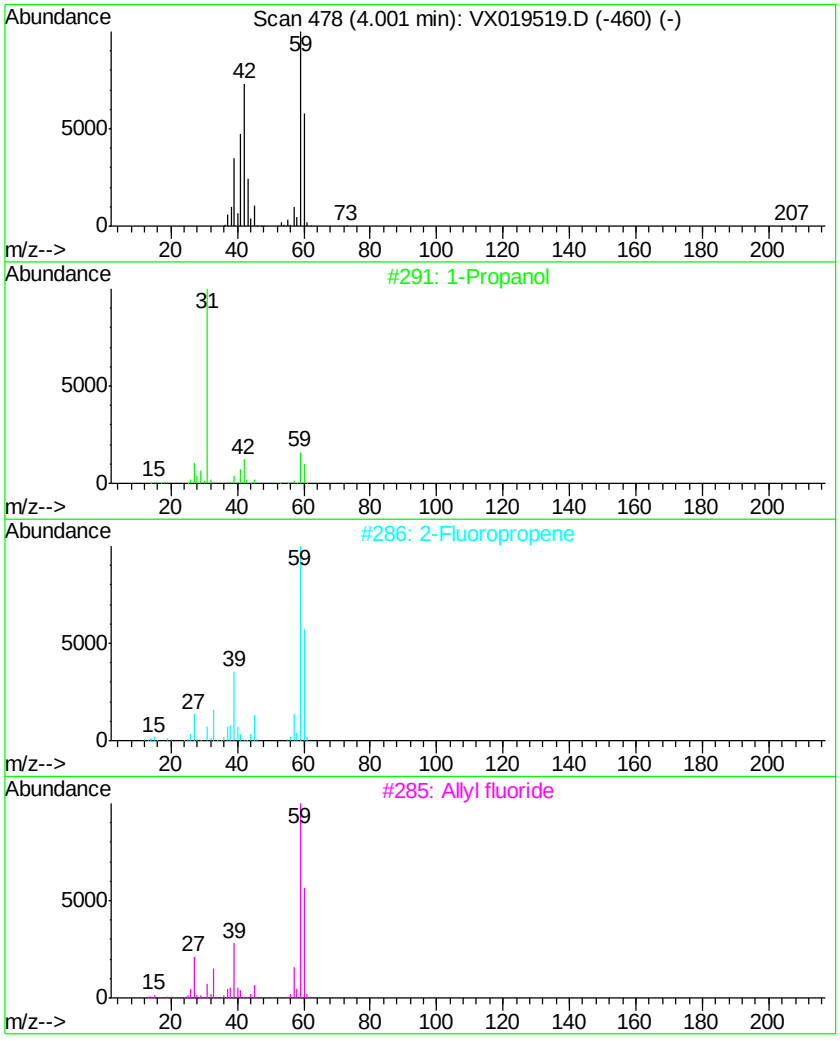
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

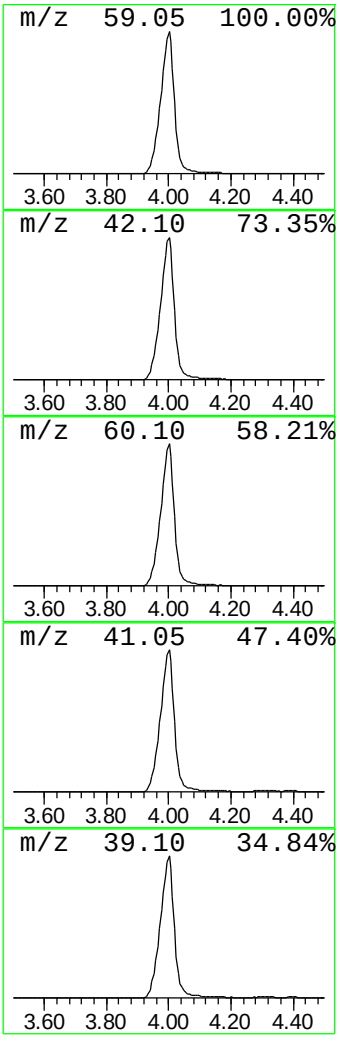
****

Peak Number 4 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.00	174.01 ug/l	2633150	Pentafluorobenzene	5.62

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	52
3	Allyl fluoride	60	C3H5F	000818-92-8	47
4	Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	9
5	Acetaldoxime	59	C2H5NO	000107-29-9	7





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Sample : L4779-02 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1641

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

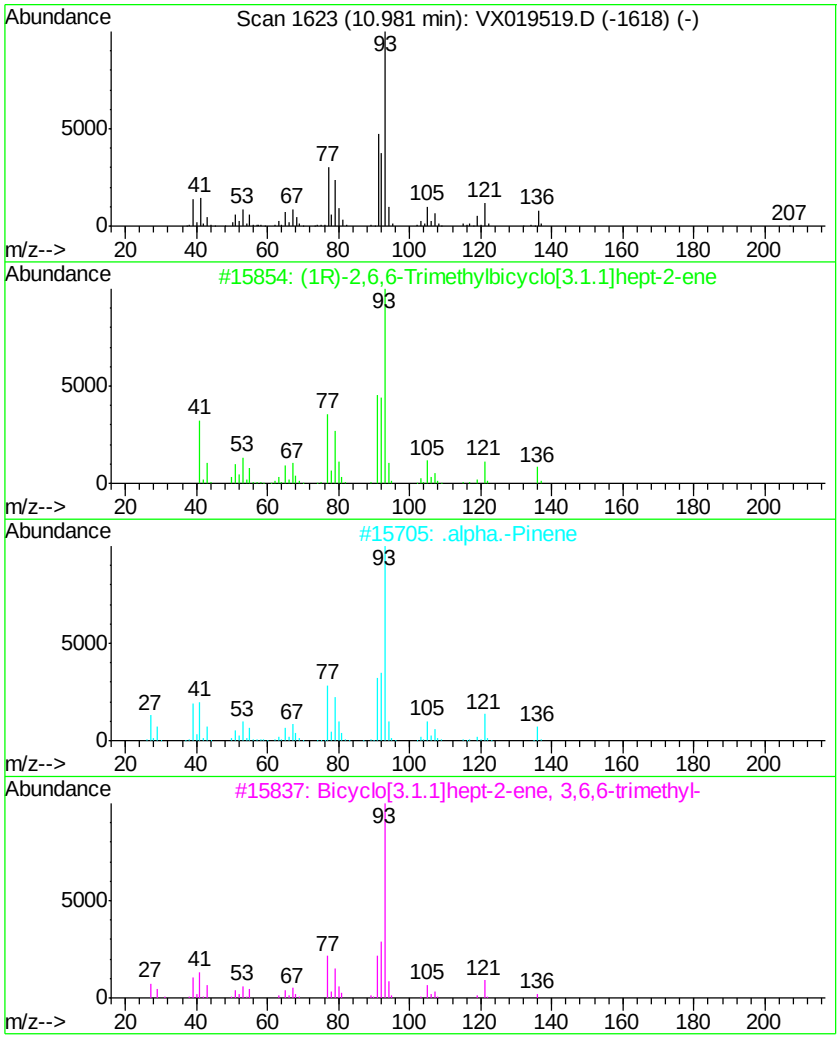
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

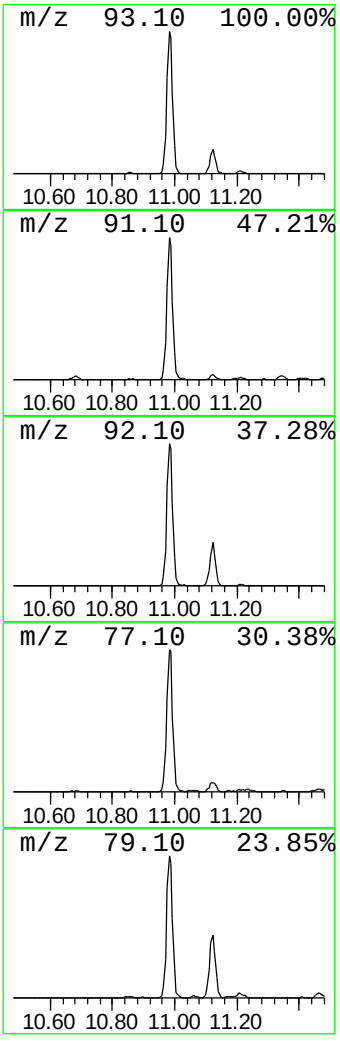
****

Peak Number 5 (1R)-2,6,6-Trimethylbicyclo... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.98	9.48 ug/l	204510	Chlorobenzene-d5	10.10

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	95
2	.alpha.-Pinene	136	C10H16	000080-56-8	95
3	Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91
4	.gamma.-Terpinene	136	C10H16	000099-85-4	91
5	(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	90





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ALS Vial : 38 Sample Multiplier: 1

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

TIC Library : C:\DATABASE\NIST11.L
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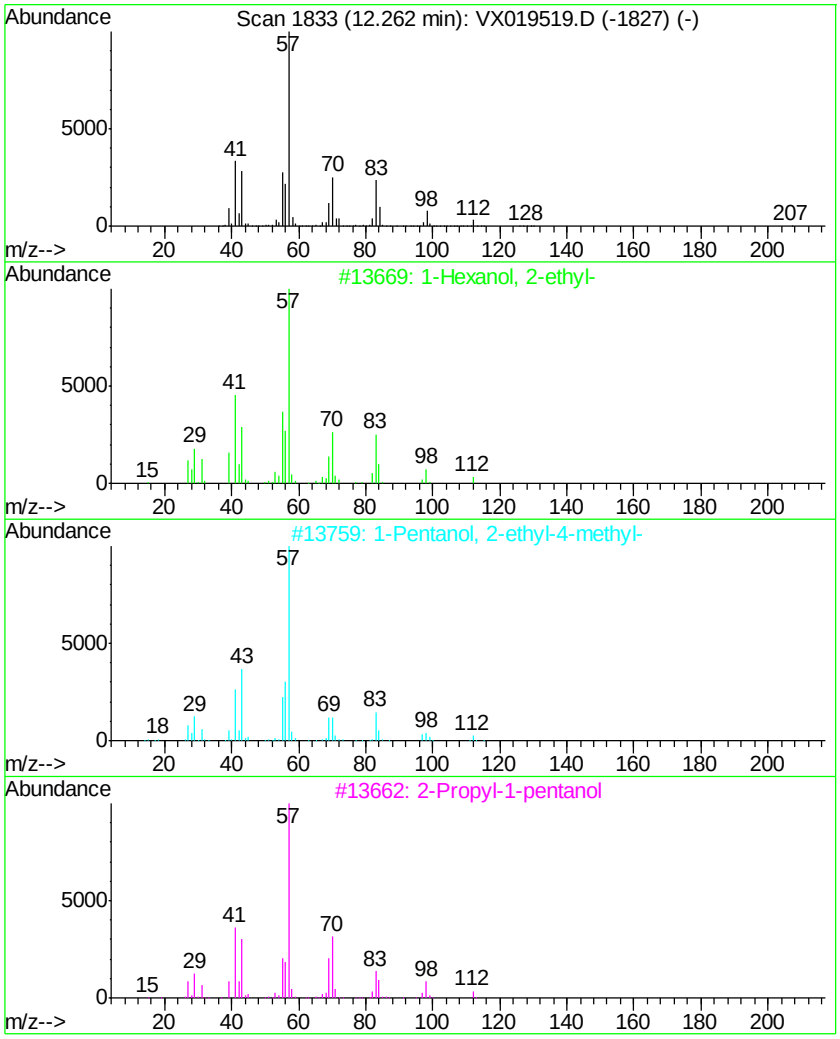
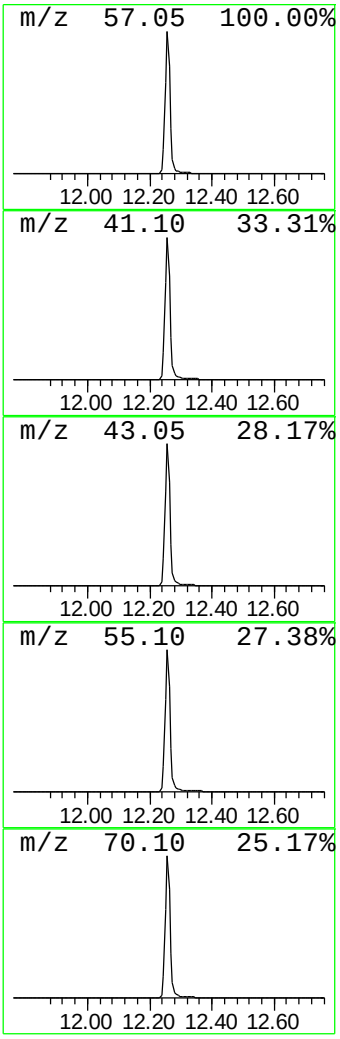
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	366.04 ug/l	7469020	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	50
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47





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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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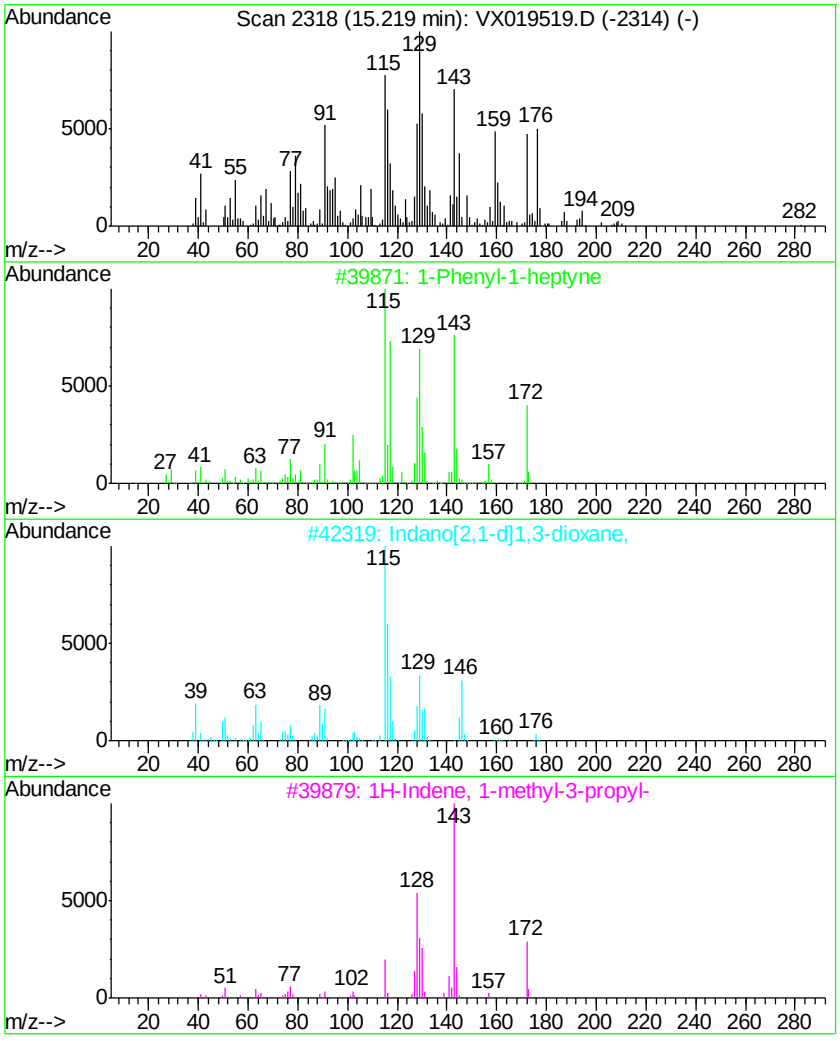
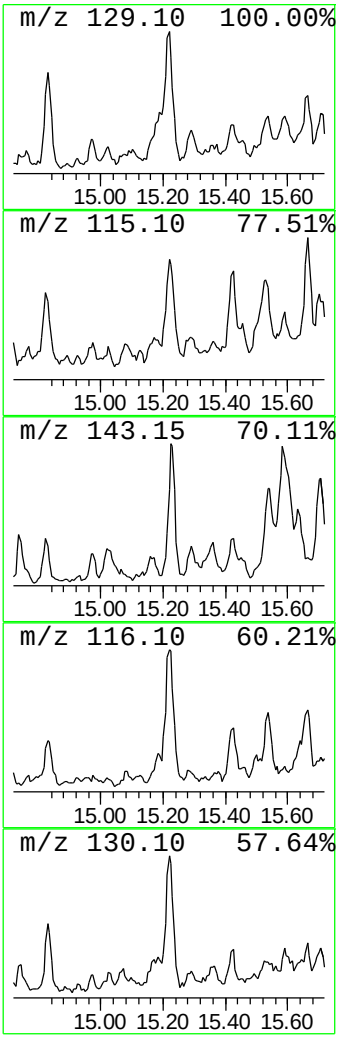
Peak Number 7 unknown15.22 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.22	10.78 ug/l	219950	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenyl-1-heptyne	172	C13H16	014374-45-9	45
2	Indano[2,1-d]1,3-dioxane,	176	C11H12O2	102688-70-0	38
3	1H-Indene, 1-methyl-3-propyl-	172	C13H16	111400-83-0	38
4	1-Naphthalenemethanol, 1,2,3,4-t...	176	C12H16O	036052-28-5	30
5	(4-Methyl-1-methylenepent-4-enyl...	172	C13H16	063942-88-1	25





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Quant Title : SW846 8260

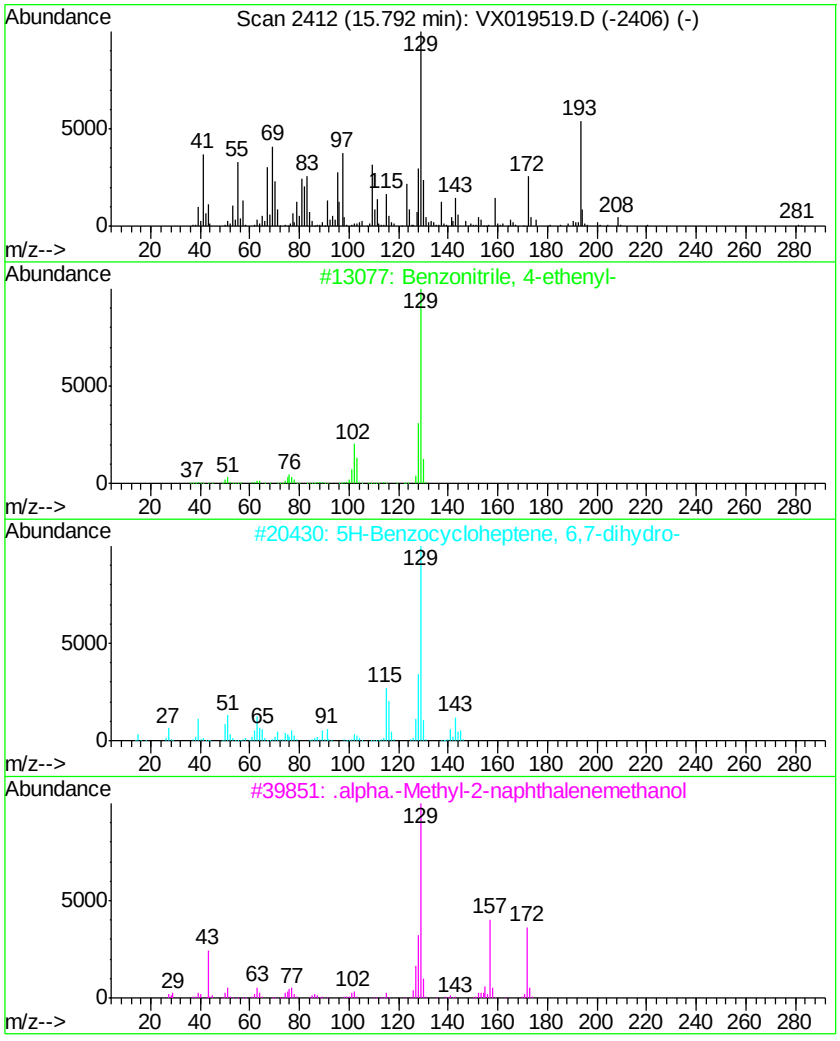
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

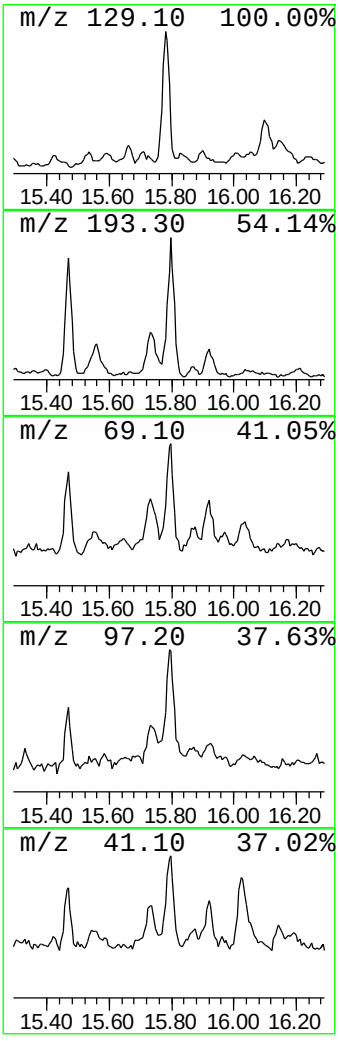
****

Peak Number 8 unknown15.79 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.79	13.43 ug/l	274005	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzonitrile, 4-ethenyl-	129	C9H7N	003435-51-6	27
2	5H-Benzocycloheptene, 6,7-dihydro-	144	C11H12	007125-62-4	27
3	.alpha.-Methyl-2-naphthalenemeth...	172	C12H12O	007228-47-9	17
4	Adipic acid, di(trans-2-methylcy...	338	C20H34O4	1000324-75-9	16
5	2-Pentanone, 4-cyclohexylidene-3...	222	C15H26O	313253-65-5	16





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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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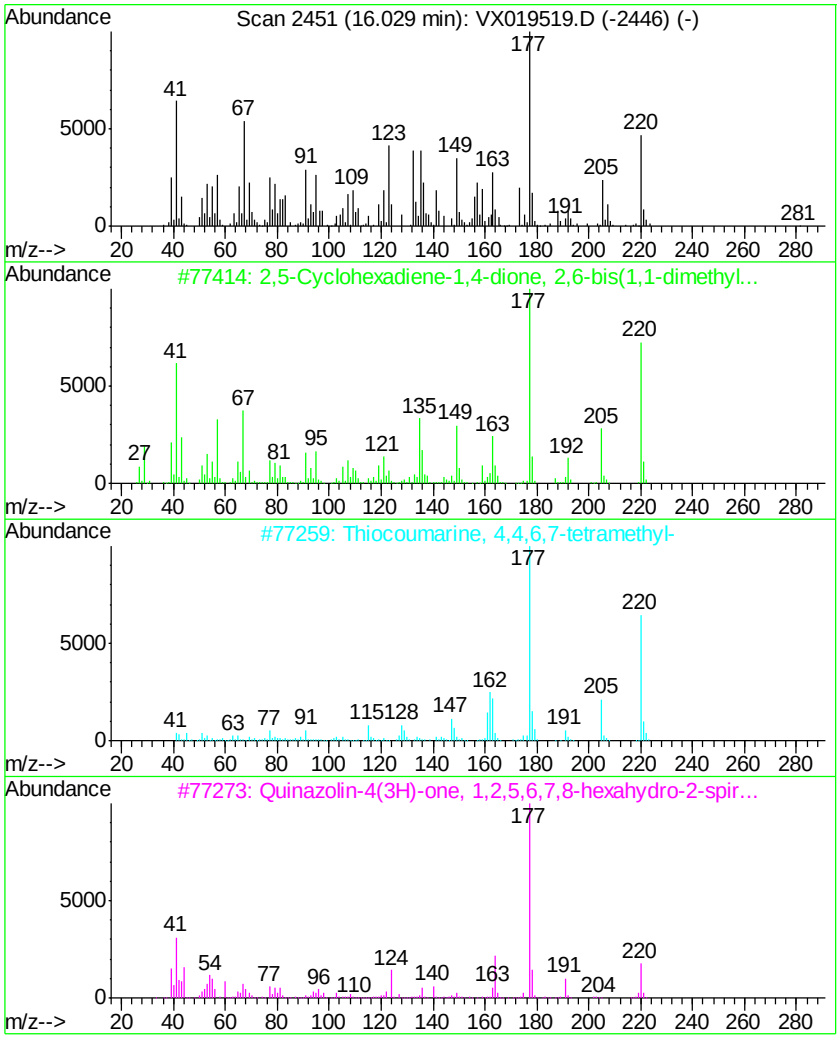
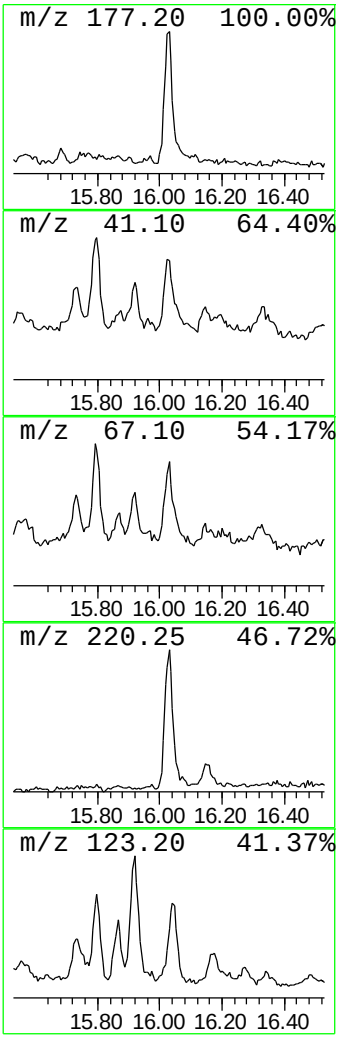
Peak Number 9 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	10.86 ug/l	221545	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	95
2	Thiocoumarine, 4,4,6,7-tetramethyl-	220	C13H16OS	1000128-90-2	30
3	Quinazolin-4(3H)-one, 1,2,5,6,7,...	220	C13H20N2O	030152-60-4	22
4	N-Cyclohexylidene-2-carbamylcycl...	220	C13H20N2O	007149-51-1	22
5	2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	20





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112120\
Data File : VX019519.D
Acq On : 21 Nov 2020 02:00
Operator : JC/MD
Sample : L4779-02 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1641

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

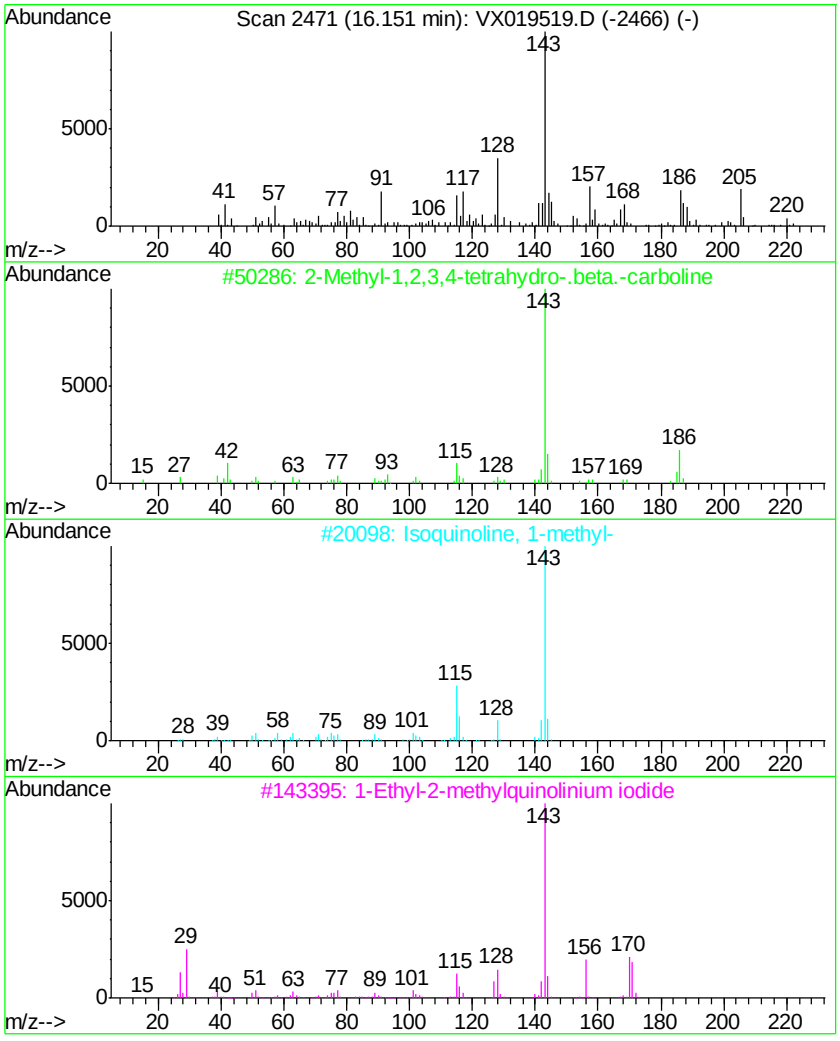
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

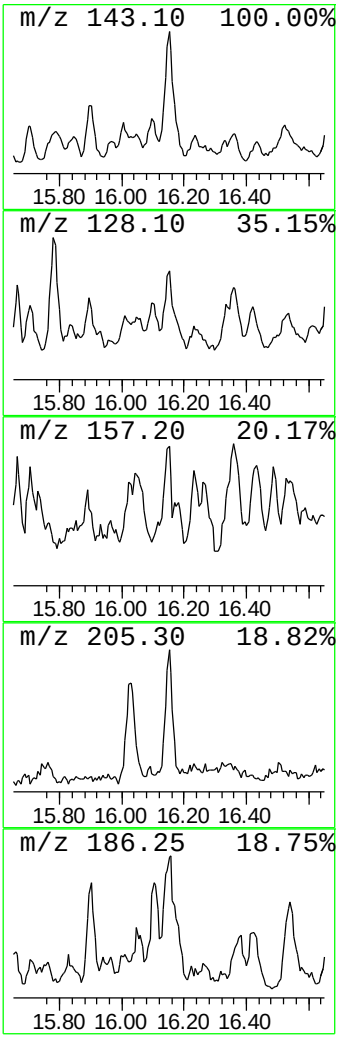
****

Peak Number 10 unknown16.15 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	6.91 ug/l	140971	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methyl-1,2,3,4-tetrahydro-.bet...	186	C12H14N2	013100-00-0	38
2	Isoquinoline, 1-methyl-	143	C10H9N	001721-93-3	35
3	1-Ethyl-2-methylquinolinium iodide	299	C12H14IN	000606-55-3	35
4	Quinolinium, 1,4-dimethyl-, iodide	285	C11H12IN	016859-86-2	35
5	1,2,3-Trimethylindene	158	C12H14	004773-83-5	32





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX112120\
Data File : VX019519.D
Acq On : 21 Nov 2020 02:00
Operator : JC/MD
Sample : L4779-02 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 1641

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
Acetaldehyde	1.47	13.7	ug/l	206983	1	5.62	756595	50.0
Ethanol	2.18	65.9	ug/l	997078	1	5.62	756595	50.0
Propanal	2.33	15.9	ug/l	240217	1	5.62	756595	50.0
1-Propanol	4.00	174.0	ug/l	2633150	1	5.62	756595	50.0
(1R)-2,6,6-Trimet...	10.98	9.5	ug/l	204510	3	10.10	1078320	50.0
1-Hexanol, 2-ethyl-	12.26	366.0	ug/l	7469020	4	12.06	1020240	50.0
unknown15.22	15.22	10.8	ug/l	219950	4	12.06	1020240	50.0
unknown15.79	15.79	13.4	ug/l	274005	4	12.06	1020240	50.0
2,5-Cyclohexadien...	16.03	10.9	ug/l	221545	4	12.06	1020240	50.0
unknown16.15	16.15	6.9	ug/l	140971	4	12.06	1020240	50.0