LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX061920\
Data File : VX016893.D
Acq On : 19 Jun 2020 20:24
Operator : JC/SP
Sample : L3054-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 218

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\82X061820W.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	2.087	158	164	174	rBV	179046	316930	1.80%	0.548%
2	2.416	211	218	235	rBV	6278387	10818864	61.48%	18.706%
3	2.575	236	244	268	rVB	1304905	2497172	14.19%	4.318%
4	4.635	571	582	597	rBV	185453	535718	3.04%	0.926%
5	5.464	707	718	732	rBV2	141430	407845	2.32%	0.705%
6	5.629	732	745	763	rVV	230476	646923	3.68%	1.119%
7	6.031	801	811	819	rBV	137864	367626	2.09%	0.636%
8	6.830	931	942	954	rBV	351604	845837	4.81%	1.462%
9	7.306	1006	1020	1034	rBV	6831675	17598620	100.00%	30.428%
10	7.519	1052	1055	1081	rVB2	57897	179532	1.02%	0.310%
11	8.622	1230	1236	1242	rBV	242557	387937	2.20%	0.671%
12	8.696	1242	1248	1254	rVV	743033	1152544	6.55%	1.993%
13	8.763	1254	1259	1265	rVB	314685	488705	2.78%	0.845%
14	9.080	1303	1311	1340	rBV	4966376	7515882	42.71%	12.995%
15	10.098	1472	1478	1489	rVB	786439	1073883	6.10%	1.857%
16	10.342	1512	1518	1524	rVB2	139861	214801	1.22%	0.371%
17	11.122	1641	1646	1657	rVB	833393	1075023	6.11%	1.859%
18	11.317	1673	1678	1685	rBV2	102009	189265	1.08%	0.327%
19	11.927	1772	1778	1786	rVV2	757618	1368365	7.78%	2.366%
20	12.061	1795	1800	1806	rVB	1081243	1344894	7.64%	2.325%
21	12.256	1827	1832	1837	rBV	1121208	1603281	9.11%	2.772%
22	12.323	1837	1843	1845	rBV3	840136	1554281	8.83%	2.687%
23	12.396	1852	1855	1862	rVV2	194833	323640	1.84%	0.560%
24	13.304	2000	2004	2007	rBV	314028	368005	2.09%	0.636%
25	13.457	2026	2029	2038	rVB5	94152	187414	1.06%	0.324%
26	13.597	2038	2052	2054	rBV3	96262	304811	1.73%	0.527%
27	13.628	2054	2057	2059	rVV2	126897	186580	1.06%	0.323%
28	13.664	2059	2063	2069	rVV2	137218	334672	1.90%	0.579%
29	13.737	2070	2075	2078	rVV2	178963	335778	1.91%	0.581%
30	13.810	2084	2087	2090	rVV2	116894	186242	1.06%	0.322%
31	13.878	2093	2098	2105	rVV2	204378	409659	2.33%	0.708%
32	14.079	2127	2131	2134	rVB	527413	564662	3.21%	0.976%
33	14.652	2222	2225	2232	rBV3	225007	290270	1.65%	0.502%
34	14.792	2244	2248	2252	rBV	676132	769480	4.37%	1.330%

LSC Area Percent Report

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ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 218

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061820W.M
Title : SW846 8260

35	15.255	2321	2324	2328	rVV	255935	312259	1.77%	0.540%
36	15.536	2365	2370	2376	rBV	536114	729306	4.14%	1.261%
37	16.438	2512	2518	2526	rVB	210388	349839	1.99%	0.605%

Sum of corrected areas: 57836545

LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX061920\
Data File : VX016893.D
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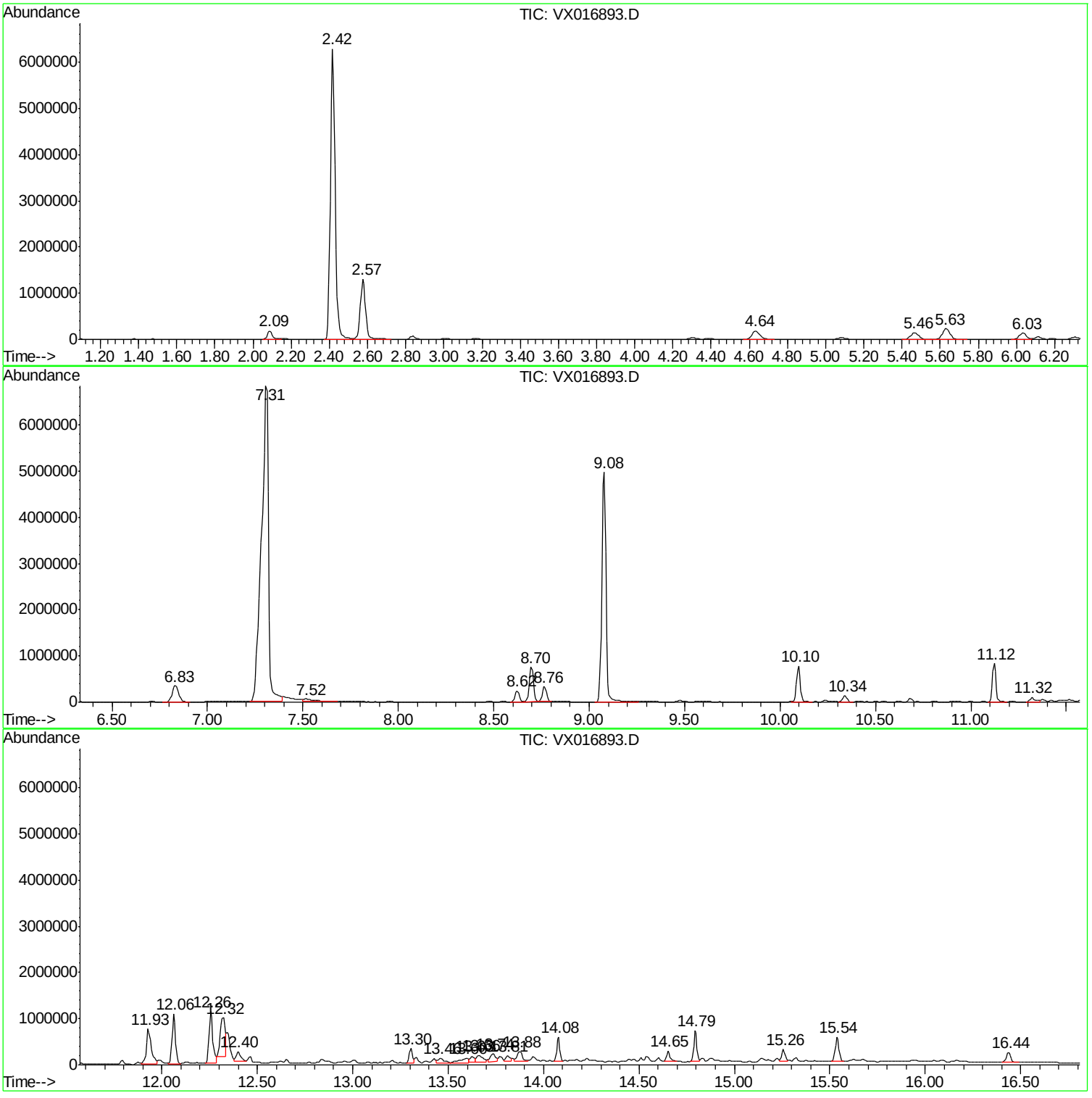
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061820W.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\VX061920\
Data File : VX016893.D
Acq On : 19 Jun 2020 20:24
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061820W.M
Quant Title : SW846 8260

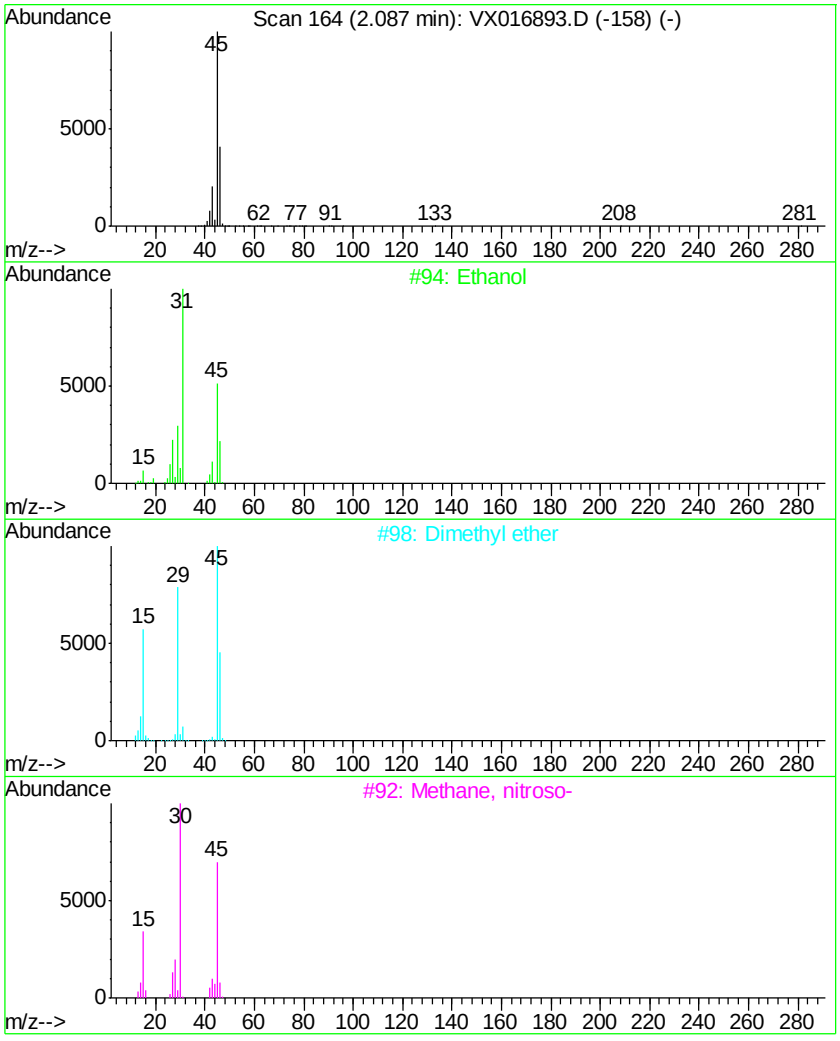
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

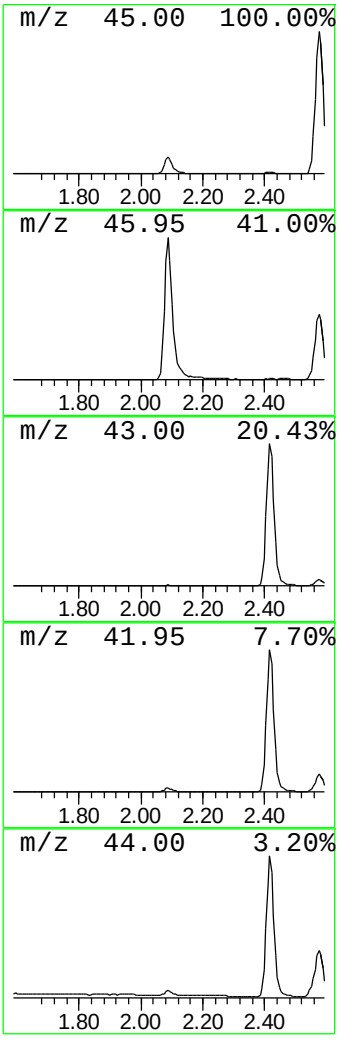
****

Peak Number 1 Ethanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.09	24.50 ug/l	316930	Pentafluorobenzene	5.63

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





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX061920\
Data File : VX016893.D
Acq On : 19 Jun 2020 20:24
Operator : JC/SP
Sample : L3054-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061820W.M
Quant Title : SW846 8260

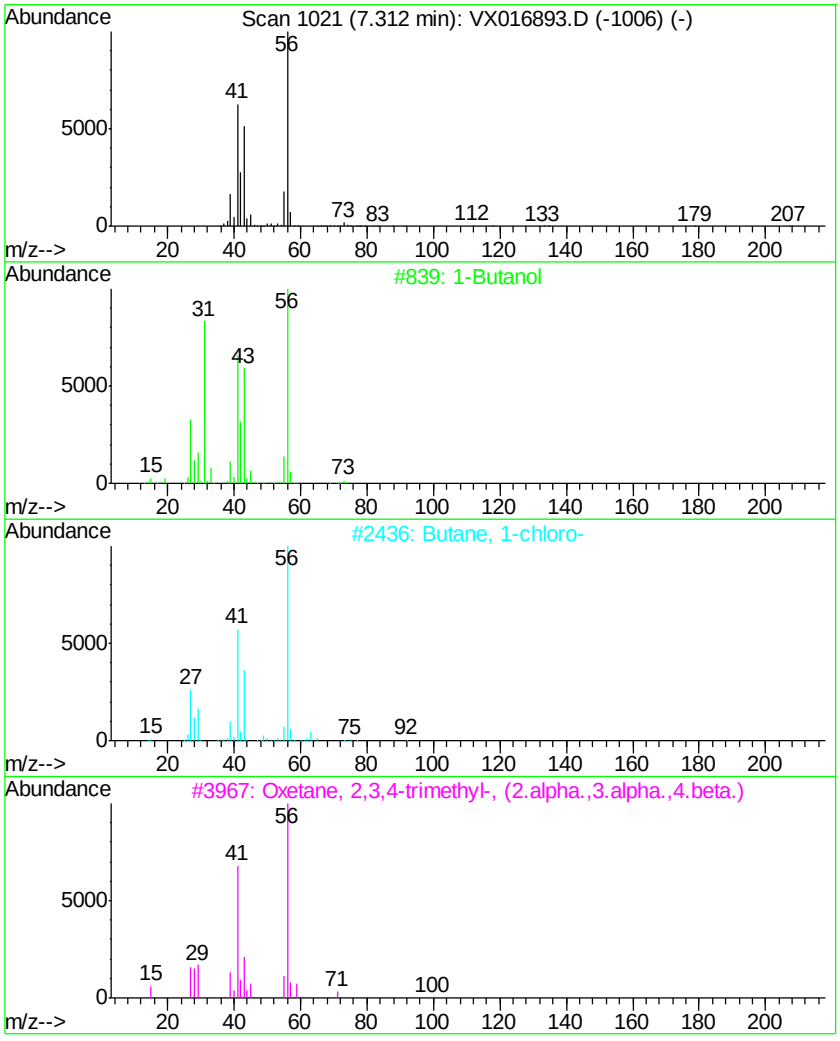
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

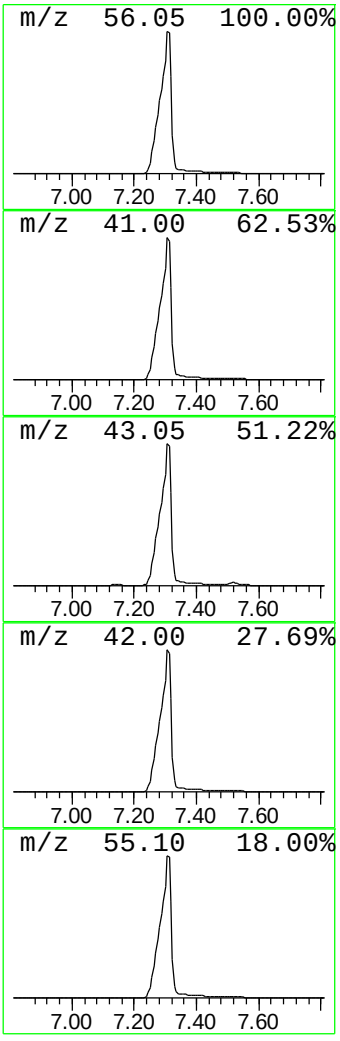
****

Peak Number 2 1-Butanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.31	1040.31 ug/l	17598600	1,4-Difluorobenzene	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	91
2	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	45
3	Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	38
4	Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX061920\
Data File : VX016893.D
Acq On : 19 Jun 2020 20:24
Operator : JC/SP
Sample : L3054-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061820W.M
Quant Title : SW846 8260

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

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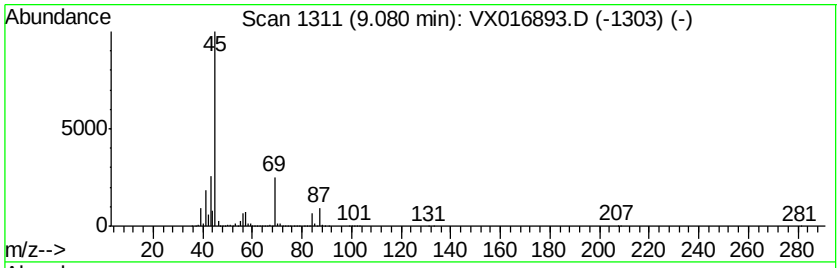
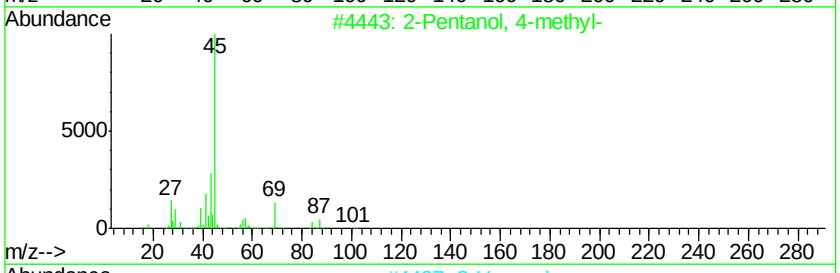
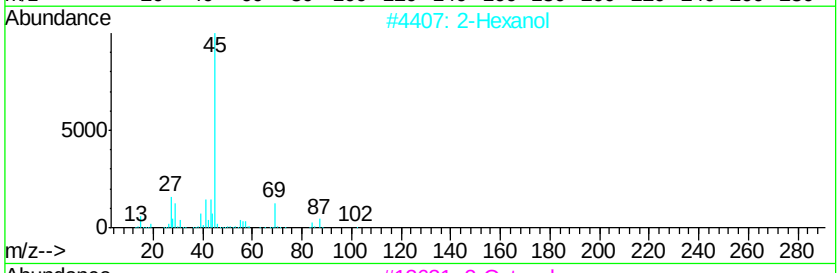
Peak Number 3 2-Pentanol, 4-methyl- Concentration Rank 2

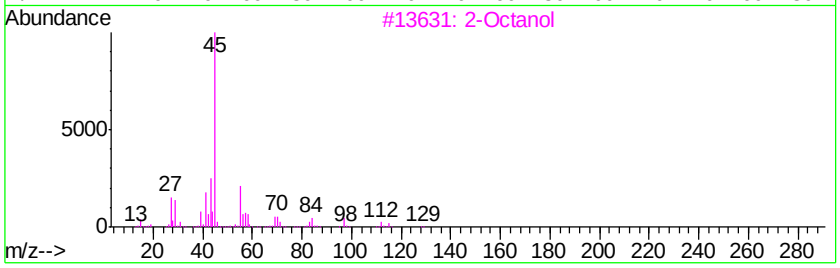
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.08	349.94 ug/l	7515880	Chlorobenzene-d5	10.10

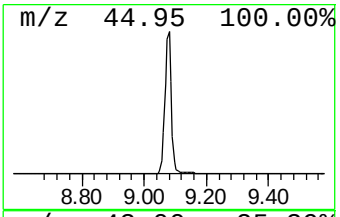
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	78
2	2-Hexanol	102	C6H14O	000626-93-7	78
3	2-Octanol	130	C8H18O	000123-96-6	72
4	2-Octanol, (R)-	130	C8H18O	005978-70-1	72
5	2-Heptanol	116	C7H16O	000543-49-7	64

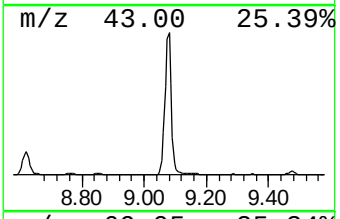


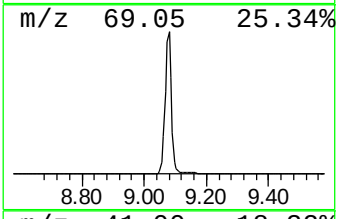


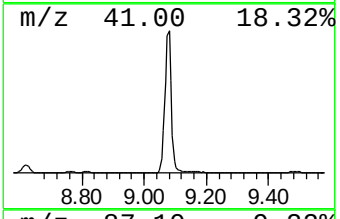


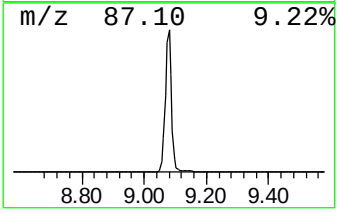












Library Search Compound Report

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ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061820W.M
Quant Title : SW846 8260

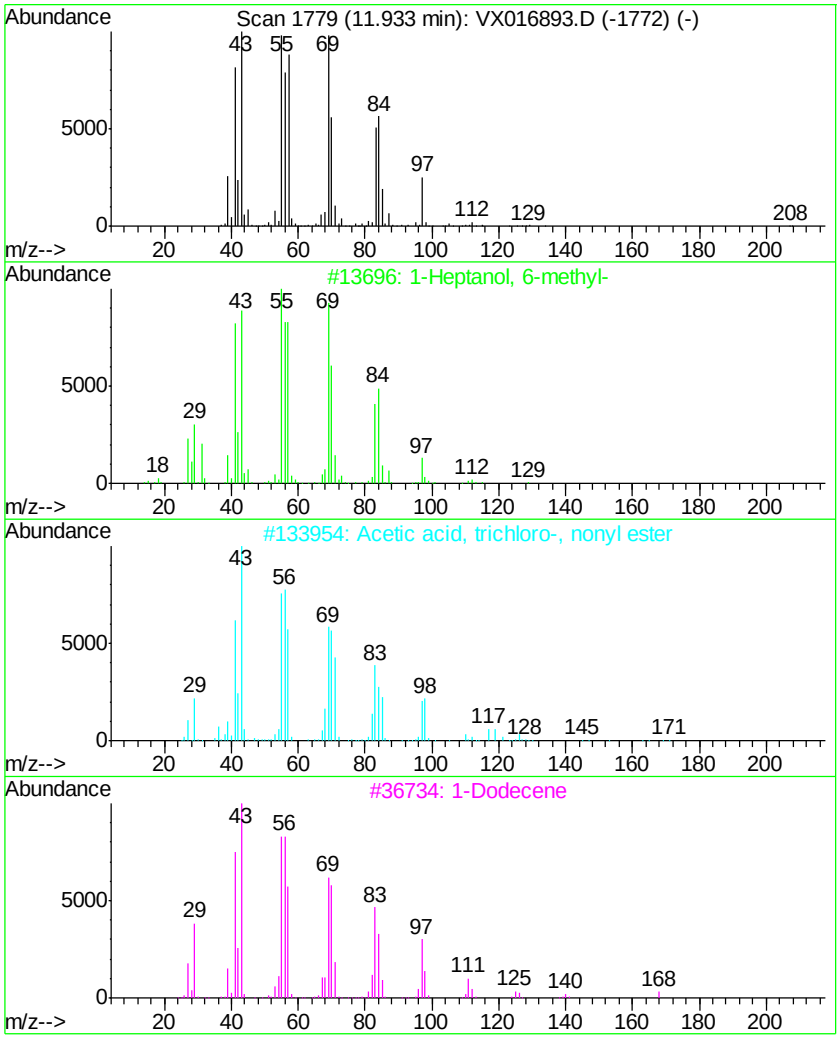
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

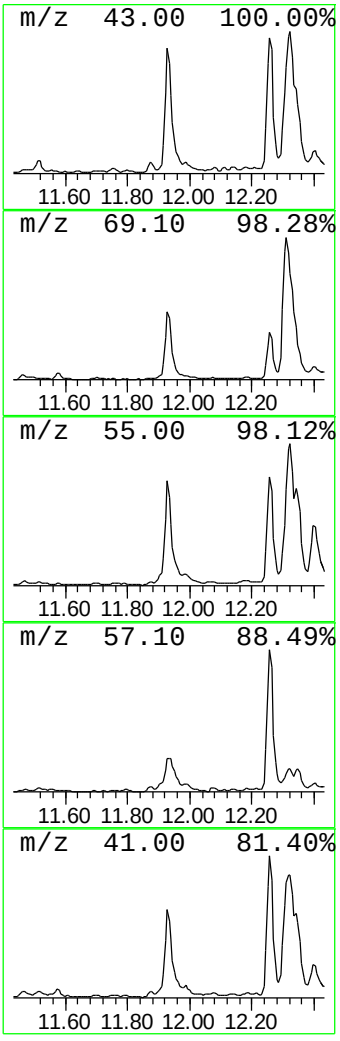
****

Peak Number 4 1-Heptanol, 6-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	50.87 ug/l	1368370	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 6-methyl-	130	C8H18O	001653-40-3	90
2	Acetic acid, trichloro-, nonyl e...	288	C11H19Cl3O2	065611-32-7	53
3	1-Dodecene	168	C12H24	000112-41-4	50
4	1-Undecanol	172	C11H24O	000112-42-5	50
5	n-Tridecan-1-ol	200	C13H28O	000112-70-9	47





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX061920\
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ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061820W.M
Quant Title : SW846 8260

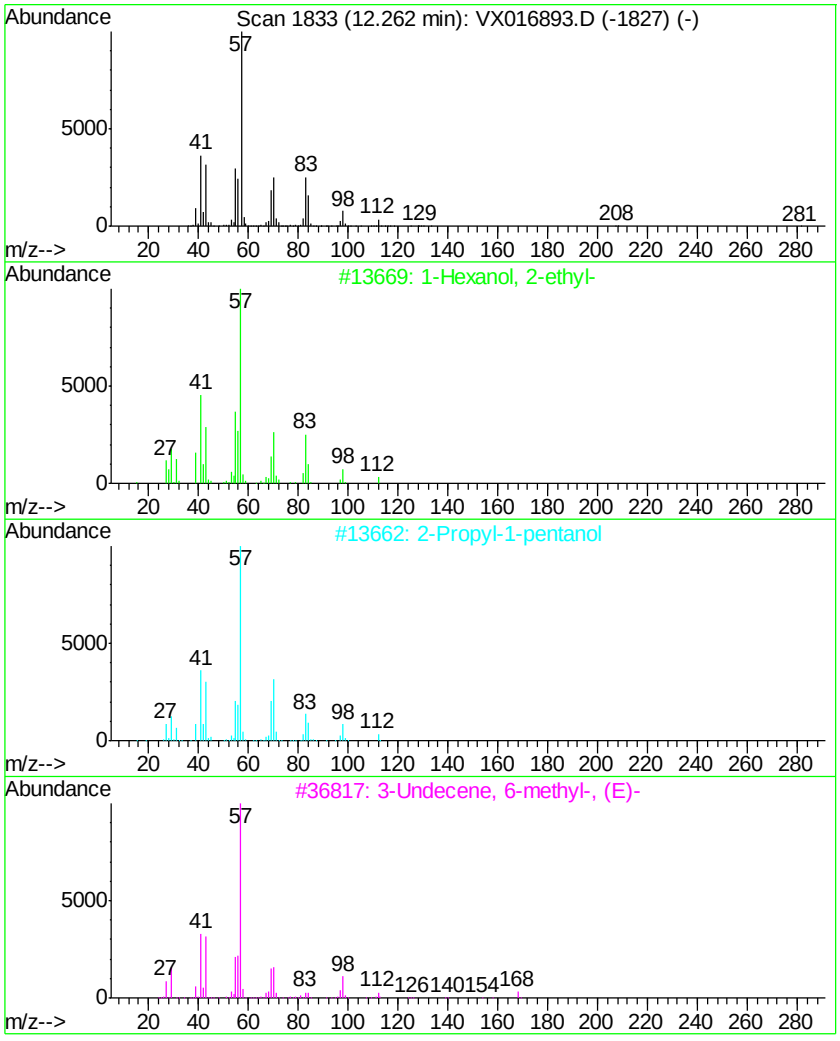
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

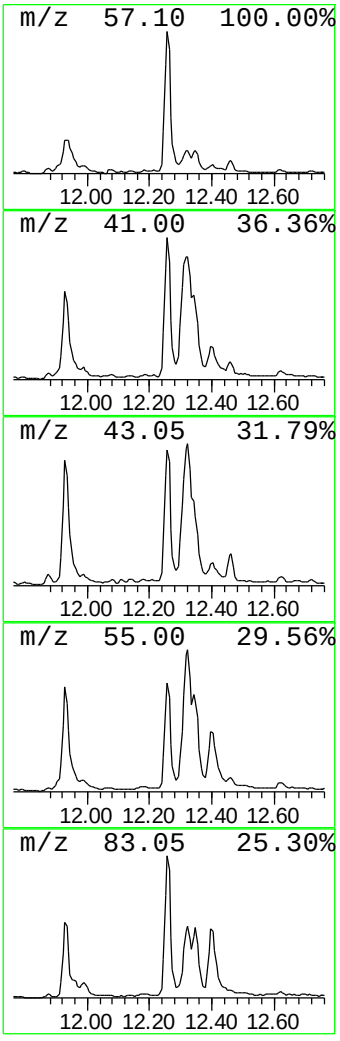
****

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	59.61 ug/l	1603280	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	78
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
3	3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	50
4	Formic acid, 2-propylpentyl ester	158	C9H18O2	1000368-74-8	47
5	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	42





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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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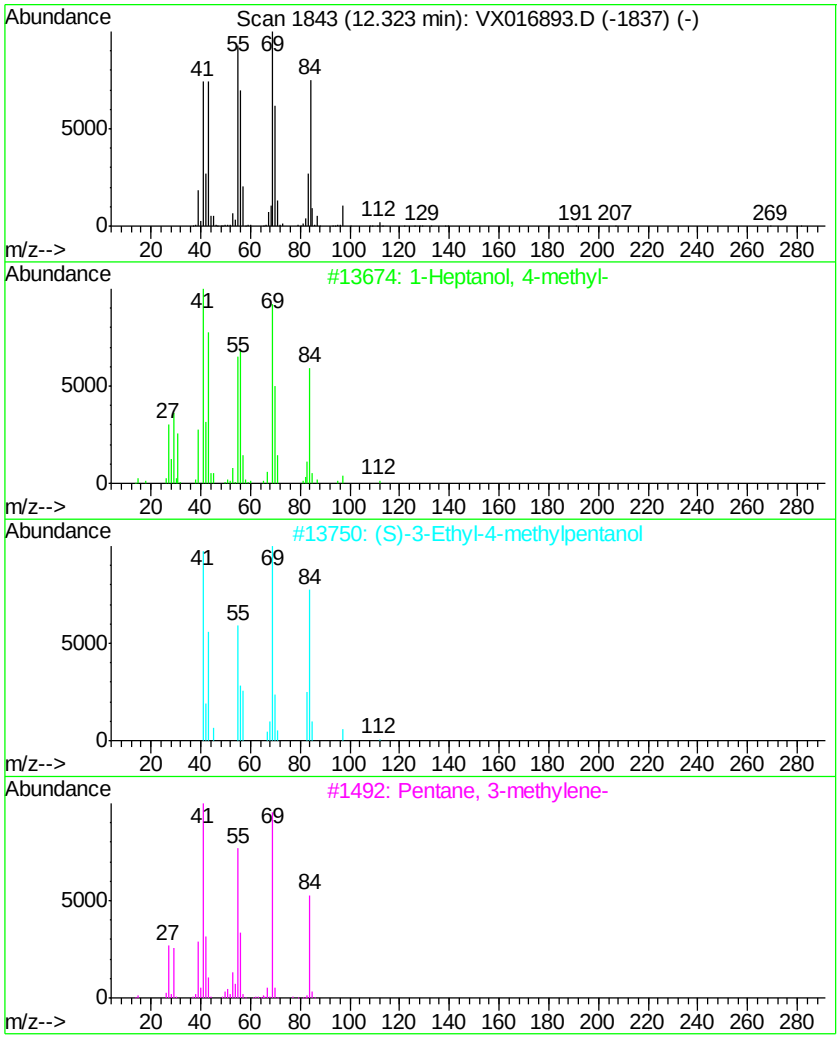
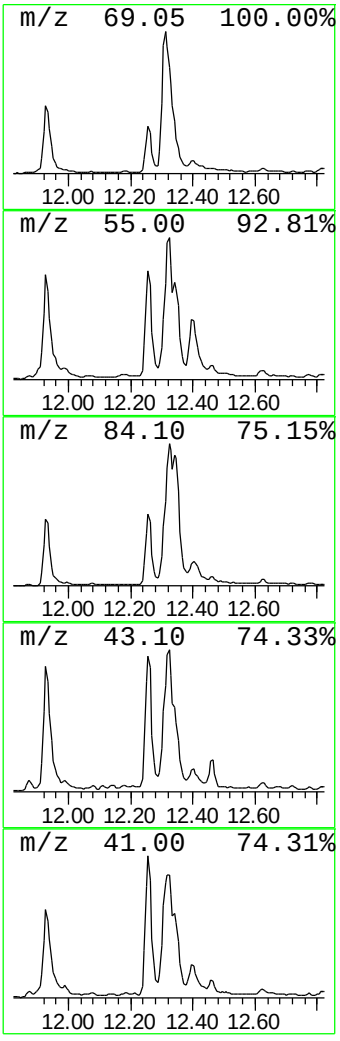
****

Peak Number 6 1-Heptanol, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	57.78 ug/l	1554280	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptanol, 4-methyl-	130	C8H18O	000817-91-4	59
2	(S)-3-Ethyl-4-methylpentanol	130	C8H18O	1000144-07-1	59
3	Pentane, 3-methylene-	84	C6H12	000760-21-4	53
4	3-Octene, (E)-	112	C8H16	014919-01-8	38
5	(S)-(+)-3-Methyl-1-pentanol	102	C6H14O	042072-39-9	38





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Sample : L3054-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061820W.M
Quant Title : SW846 8260

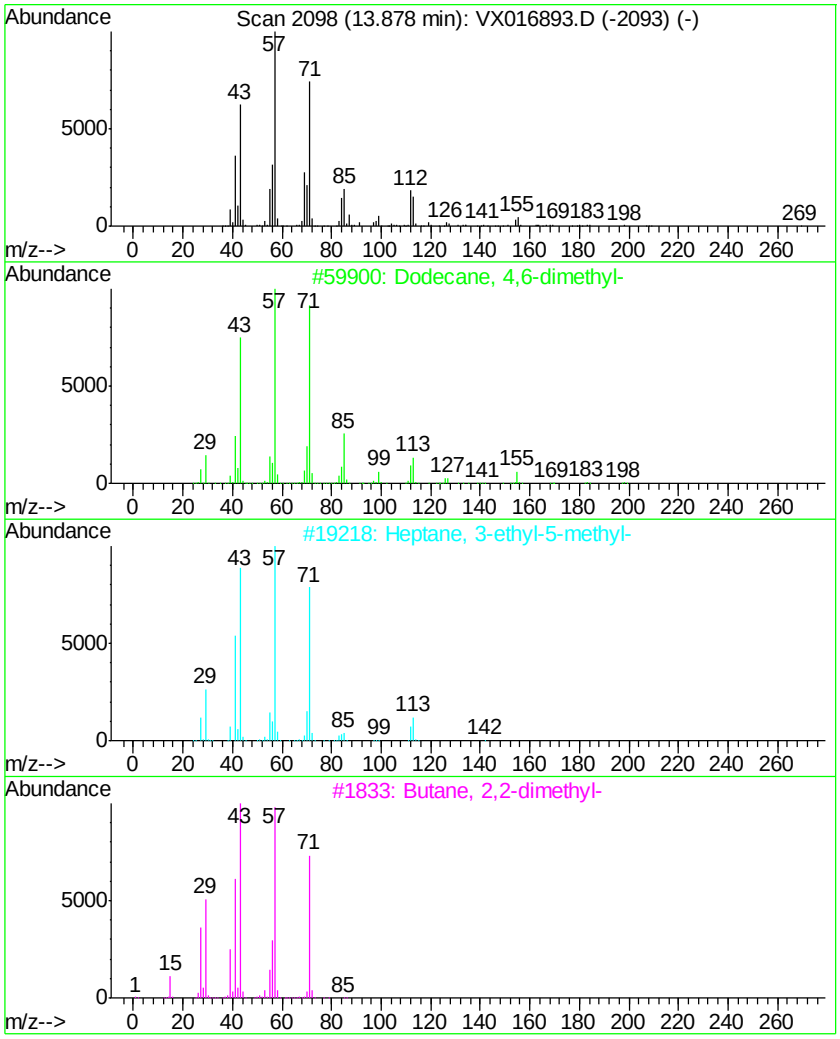
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

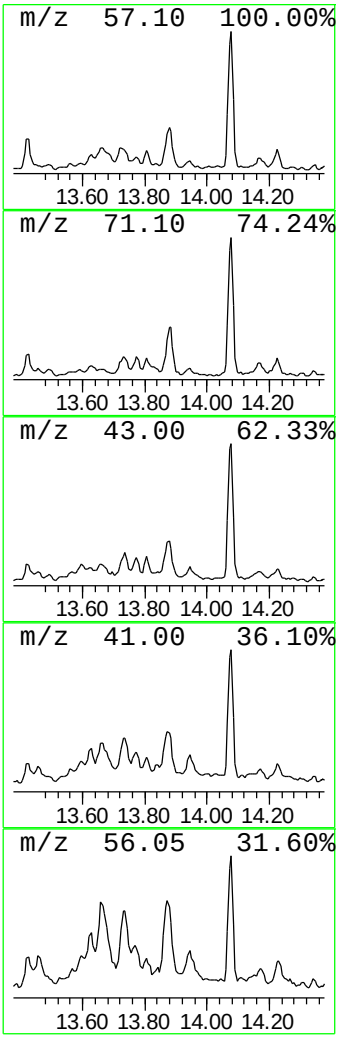
****

Peak Number 7 Dodecane, 4,6-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	15.23 ug/l	409659	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 4,6-dimethyl-	198	C14H30	061141-72-8	81
2	Heptane, 3-ethyl-5-methyl-	142	C10H22	052896-90-9	53
3	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	47
4	Hexane, 2,4,4-trimethyl-	128	C9H20	016747-30-1	47
5	Ether, 3-butenyl pentyl	142	C9H18O	034061-78-4	43





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Instrument : MSVOA_X
ClientSampleId : 218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061820W.M
Quant Title : SW846 8260

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

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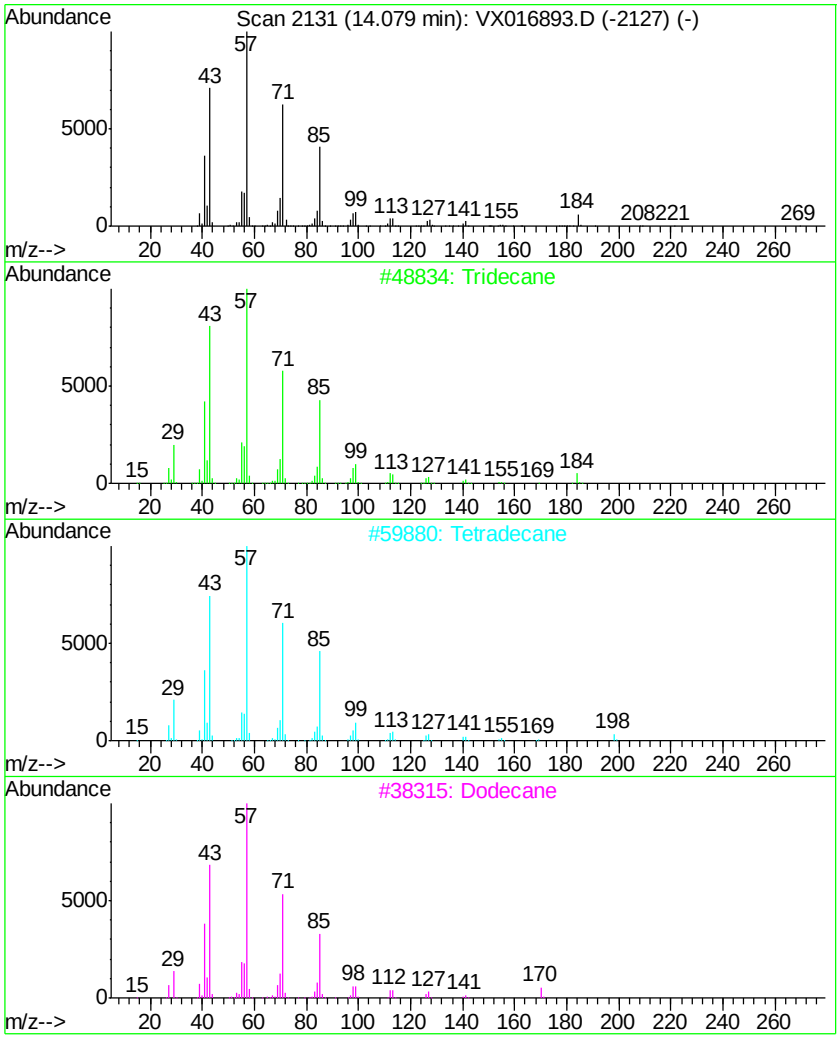
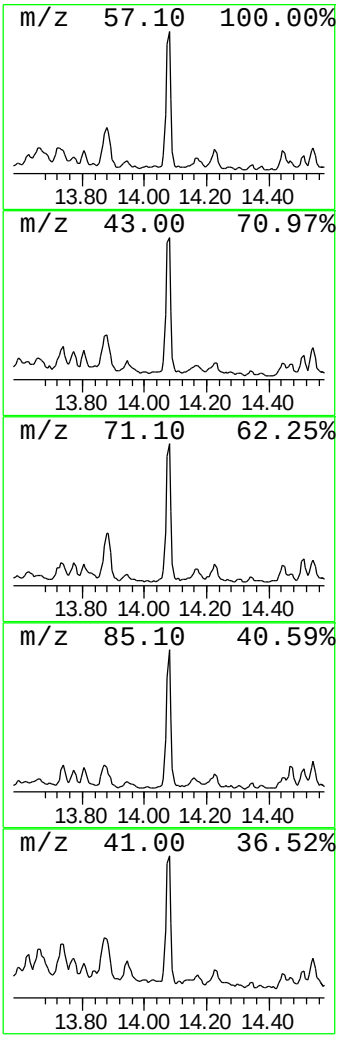
Peak Number 8 Tridecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.08	20.99 ug/l	564662	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	97
2	Tetradecane	198	C14H30	000629-59-4	86
3	Dodecane	170	C12H26	000112-40-3	86
4	Nonane	128	C9H20	000111-84-2	70
5	Hexadecane	226	C16H34	000544-76-3	64





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX061920\
Data File : VX016893.D
Acq On : 19 Jun 2020 20:24
Operator : JC/SP
Sample : L3054-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061820W.M
Quant Title : SW846 8260

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

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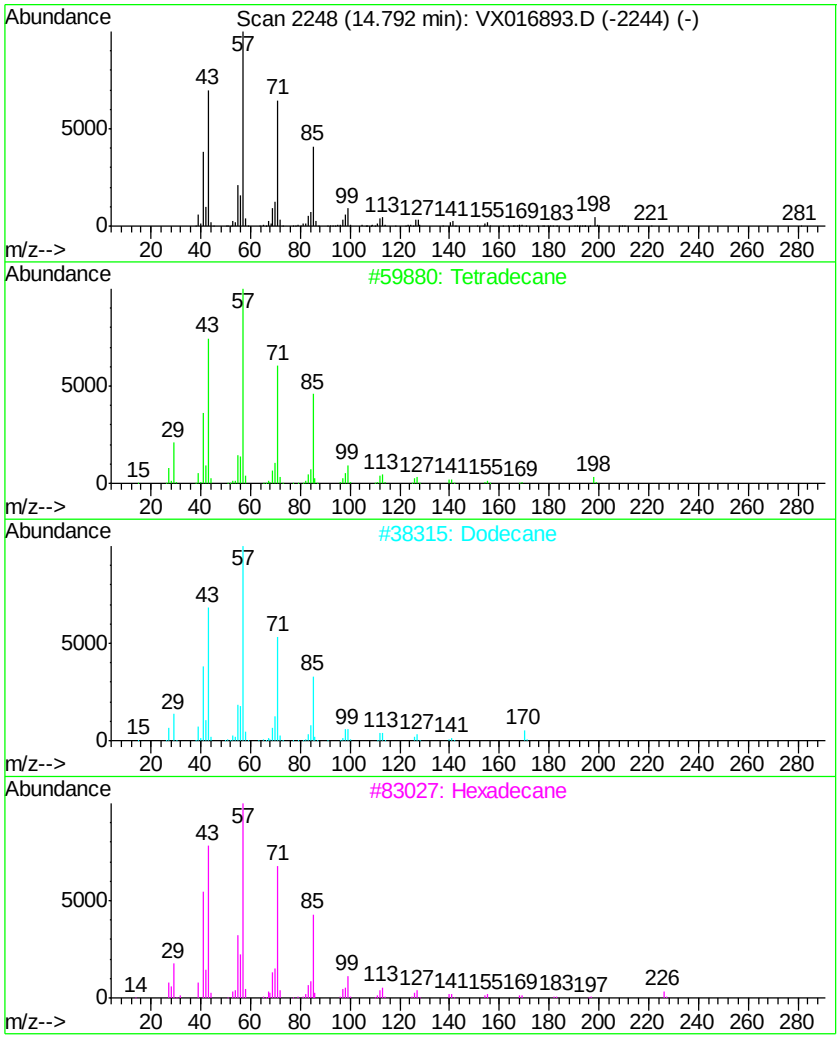
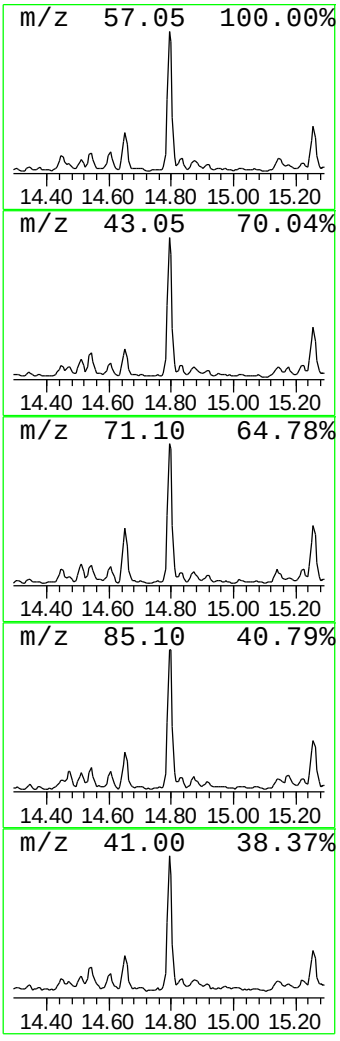
Peak Number 9 Tetradecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	28.61 ug/l	769480	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	98
2	Dodecane	170	C12H26	000112-40-3	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Tridecane	184	C13H28	000629-50-5	86
5	Pentadecane	212	C15H32	000629-62-9	86





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX061920\
Data File : VX016893.D
Acq On : 19 Jun 2020 20:24
Operator : JC/SP
Sample : L3054-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061820W.M
Quant Title : SW846 8260

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

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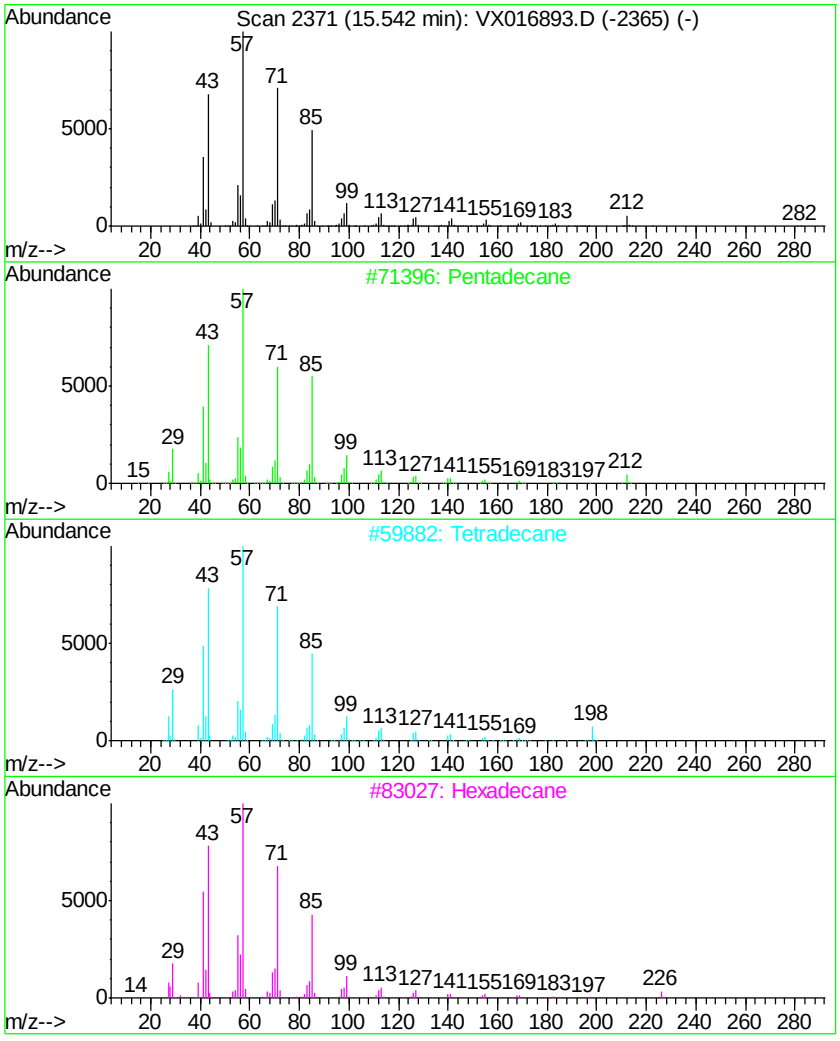
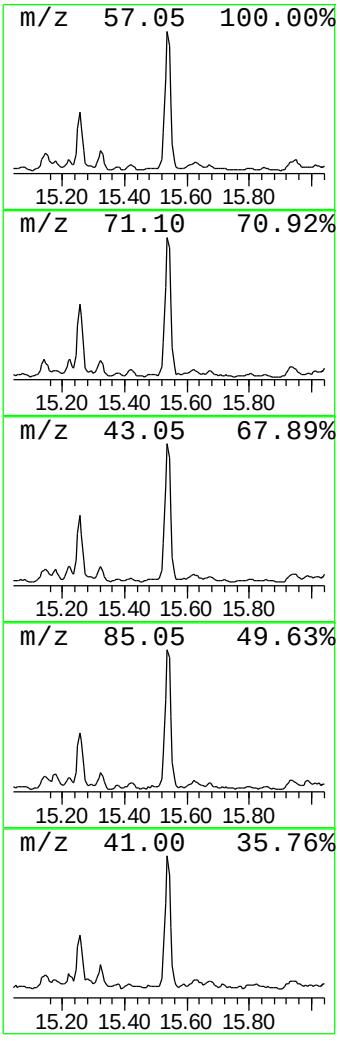
Peak Number 10 Pentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.54	27.11 ug/l	729306	1,4-Dichlorobenzene-d4	12.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	97
2	Tetradecane	198	C14H30	000629-59-4	91
3	Hexadecane	226	C16H34	000544-76-3	90
4	Heptadecane	240	C17H36	000629-78-7	87
5	Tridecane	184	C13H28	000629-50-5	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX061920\
Data File : VX016893.D
Acq On : 19 Jun 2020 20:24
Operator : JC/SP
Sample : L3054-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : 218

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X061820W.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	2.09	24.5	ug/l	316930	1	5.63	646923	50.0
1-Butanol	7.31	1040.3	ug/l	17598600	2	6.84	845837	50.0
2-Pentanol, 4-met...	9.08	349.9	ug/l	7515880	3	10.10	1073880	50.0
1-Heptanol, 6-met...	11.93	50.9	ug/l	1368370	4	12.06	1344890	50.0
1-Hexanol, 2-ethyl-	12.26	59.6	ug/l	1603280	4	12.06	1344890	50.0
1-Heptanol, 4-met...	12.32	57.8	ug/l	1554280	4	12.06	1344890	50.0
Dodecane, 4,6-dim...	13.88	15.2	ug/l	409659	4	12.06	1344890	50.0
Tridecane	14.08	21.0	ug/l	564662	4	12.06	1344890	50.0
Tetradecane	14.79	28.6	ug/l	769480	4	12.06	1344890	50.0
Pentadecane	15.54	27.1	ug/l	729306	4	12.06	1344890	50.0