LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX110122\
Data File : VX032506.D
Acq On : 01 Nov 2022 12:28
Operator : JC/MD
Sample : N5391-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31846

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\82X102622W.M
Title : SW846 8260

Signal : TIC: VX032506.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	56	60	72	rBV	423797	506832	40.76%	7.688%
2	1.605	76	85	96	rVB5	4164	14726	1.18%	0.223%
3	2.099	155	166	184	rBV	121256	398154	32.02%	6.039%
4	2.380	205	212	229	rBV	749754	1243330	100.00%	18.859%
5	2.557	231	241	256	rVB	24571	72004	5.79%	1.092%
6	2.947	293	305	315	rBV	6596	15768	1.27%	0.239%
7	3.117	323	333	343	rVB2	5635	12916	1.04%	0.196%
8	4.562	561	570	583	rBV3	8155	26862	2.16%	0.407%
9	5.385	694	705	721	rBV2	75286	220946	17.77%	3.351%
10	5.556	722	733	748	rVB	127653	361588	29.08%	5.484%
11	5.958	789	799	814	rBV	82842	216563	17.42%	3.285%
12	6.763	921	931	948	rBV	196094	460942	37.07%	6.991%
13	8.647	1234	1240	1251	rBV	391151	621235	49.97%	9.423%
14	10.055	1465	1471	1481	rBV	400088	531046	42.71%	8.055%
15	11.079	1634	1639	1648	rBV	358701	460954	37.07%	6.992%
16	11.421	1691	1695	1703	rBV	17175	23978	1.93%	0.364%
17	12.024	1788	1794	1801	rBV	408431	507293	40.80%	7.695%
18	12.219	1821	1826	1843	rBV	297774	432587	34.79%	6.561%
19	13.152	1973	1979	1993	rBV	151039	225774	18.16%	3.424%
20	14.042	2120	2125	2131	rBV3	18207	25878	2.08%	0.393%
21	14.756	2238	2242	2246	rBV	29858	32468	2.61%	0.492%
22	15.103	2293	2299	2302	rBV7	5652	12510	1.01%	0.190%
23	15.213	2314	2317	2320	rVV	19569	24361	1.96%	0.370%
24	15.493	2358	2363	2367	rBV	44254	61085	4.91%	0.927%
25	16.030	2448	2451	2456	rVB4	8051	13332	1.07%	0.202%
26	16.377	2501	2508	2514	rVB	40886	69780	5.61%	1.058%

Sum of corrected areas: 6592912

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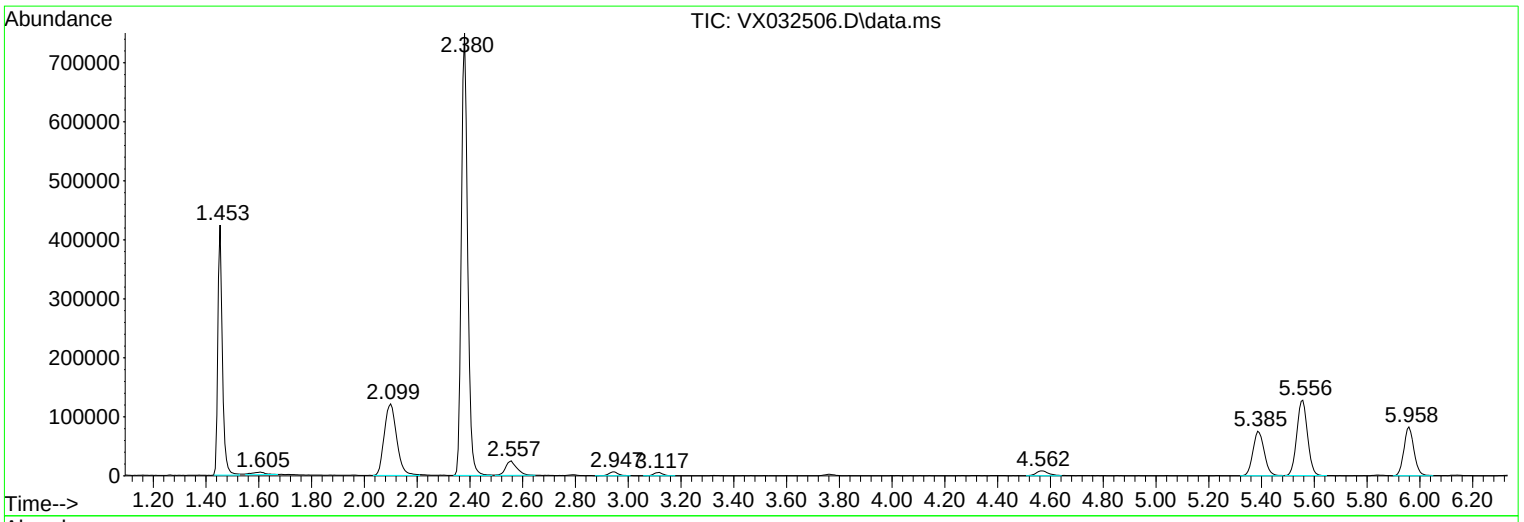
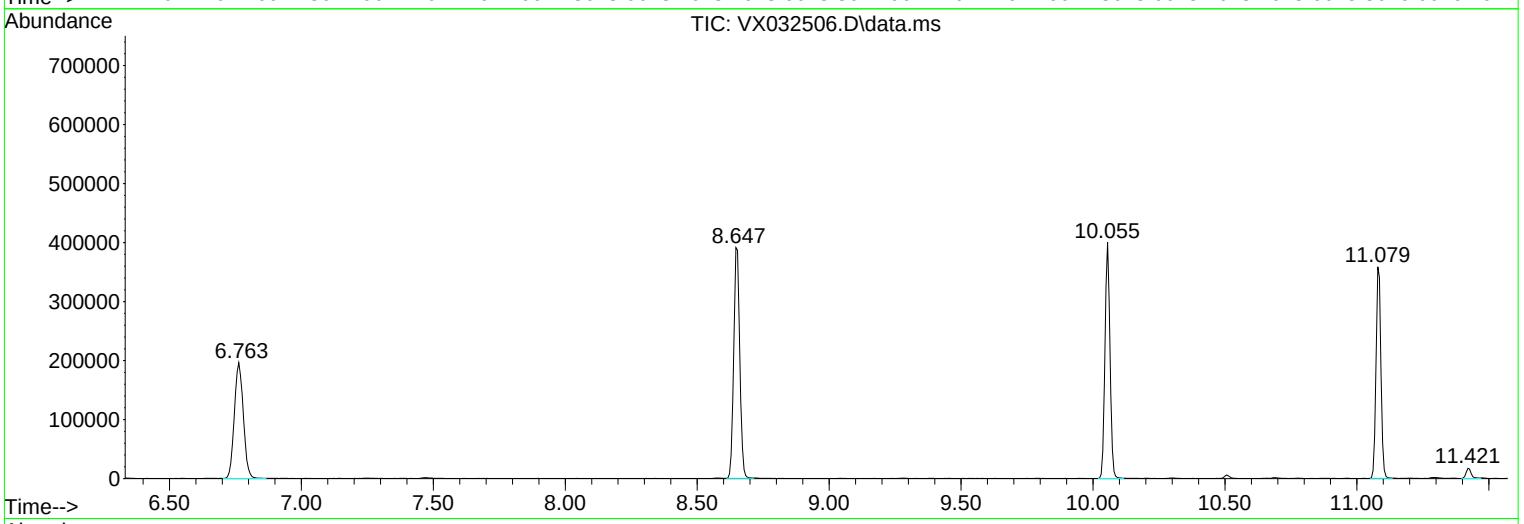
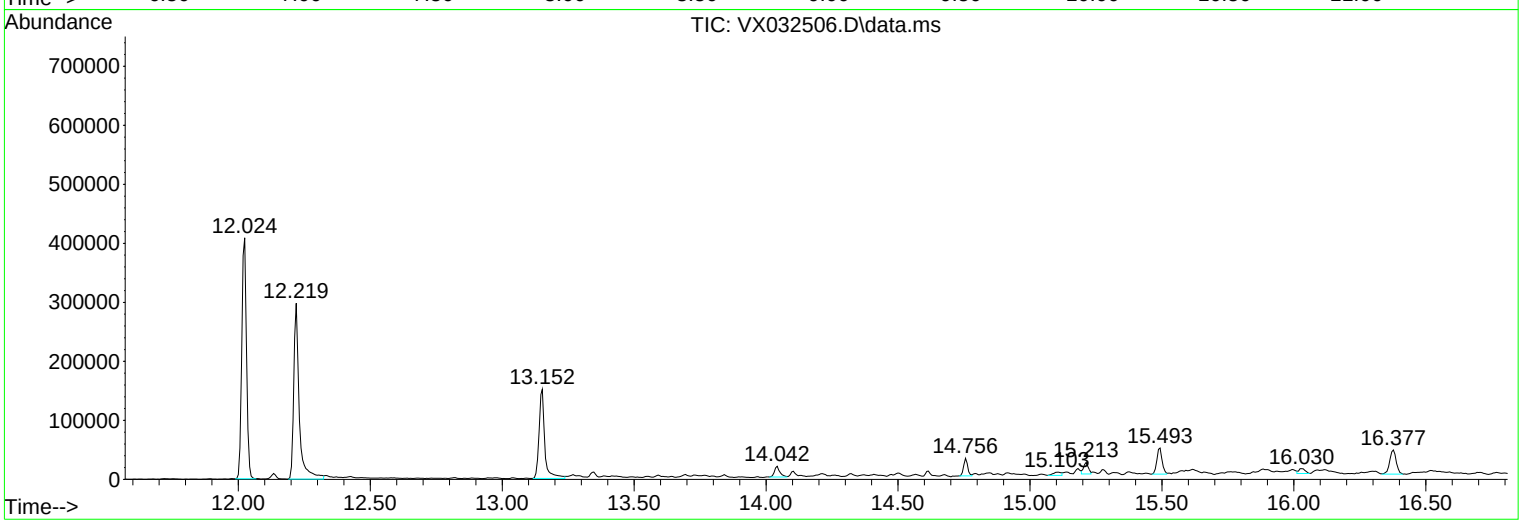
ClientSampleId :
31846

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

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







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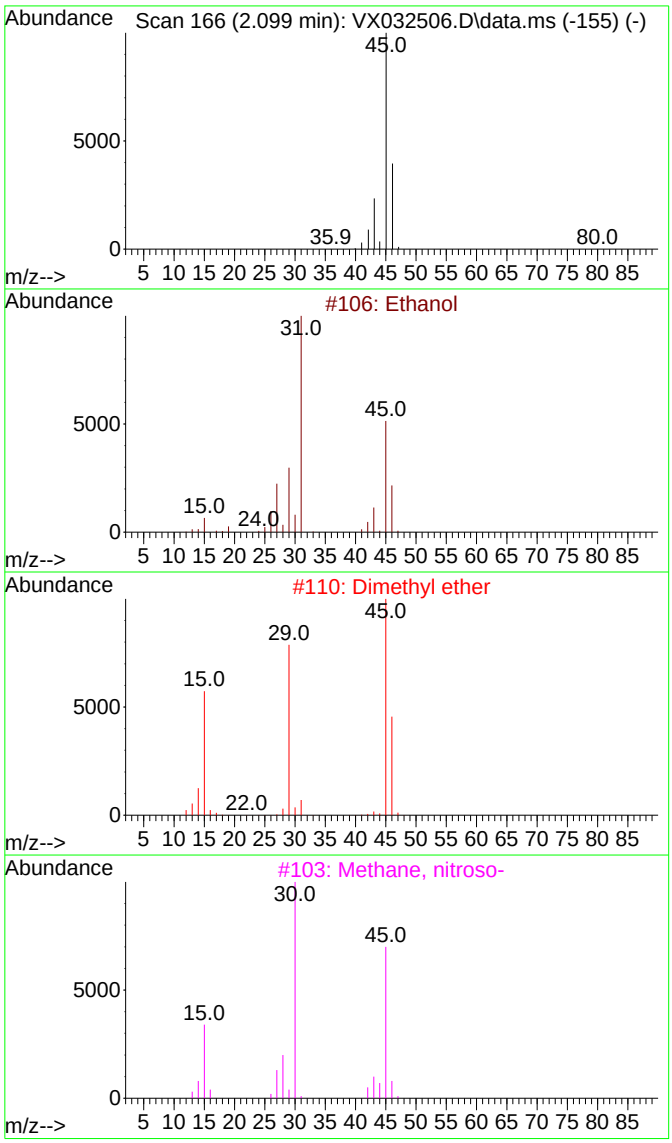
Quant Title : SW846 8260

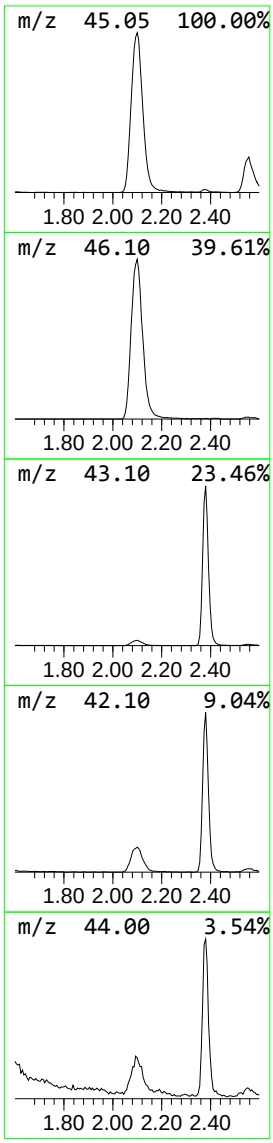
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.099	55.06 ug/l	398154	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	74
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 : VX032506.D
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Operator : JC/MD
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
31846

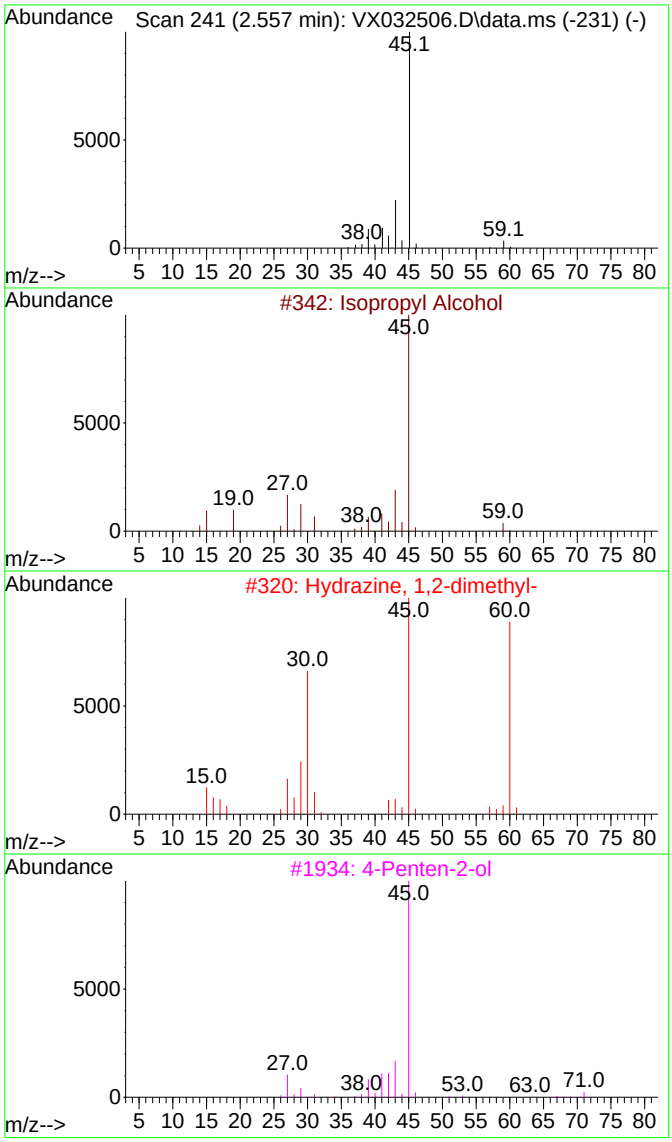
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

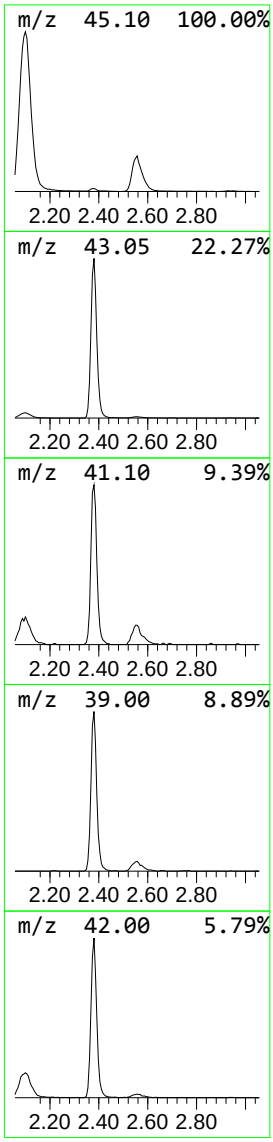
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Isopropyl Alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.557	9.96 ug/l	72004	Pentafluorobenzene	5.556

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3	4-Penten-2-ol	86	C5H10O	000625-31-0	9
4	Formamide	45	CH3NO	000075-12-7	4
5	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	4





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Instrument :
MSVOA_X
ClientSampleId :
31846

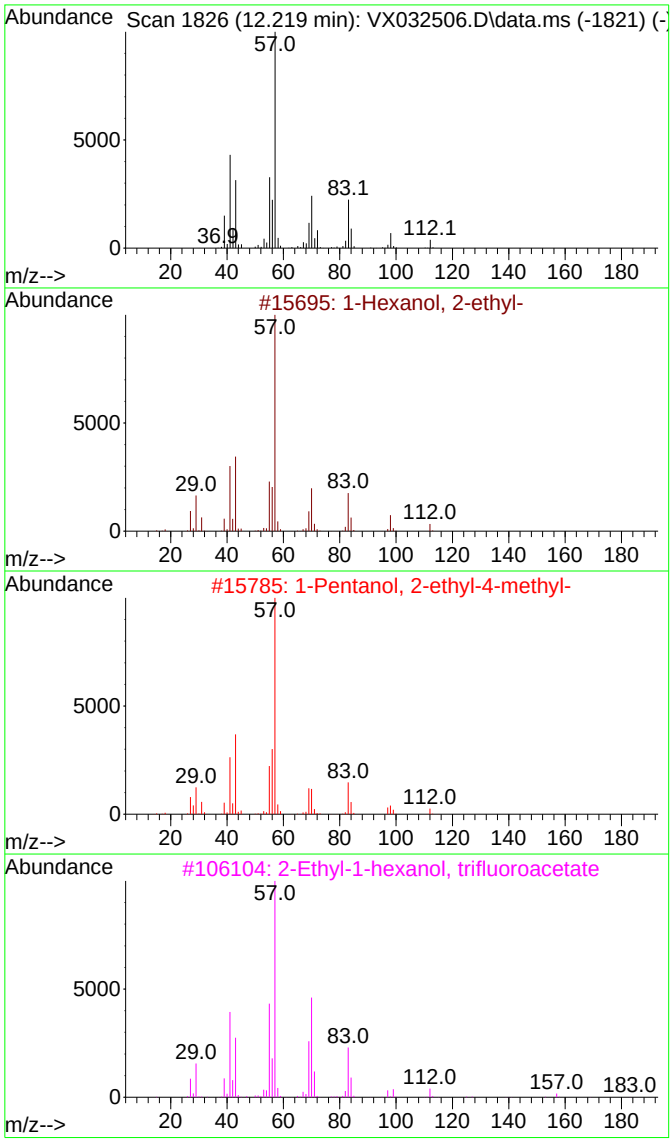
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

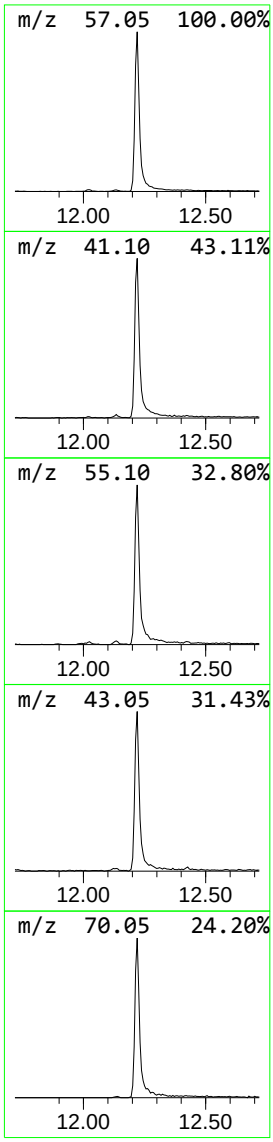
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	42.64 ug/l	432587	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	83
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
3	2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	053800-08-1	50
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5	Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	50





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Instrument :
MSVOA_X
ClientSampleId :
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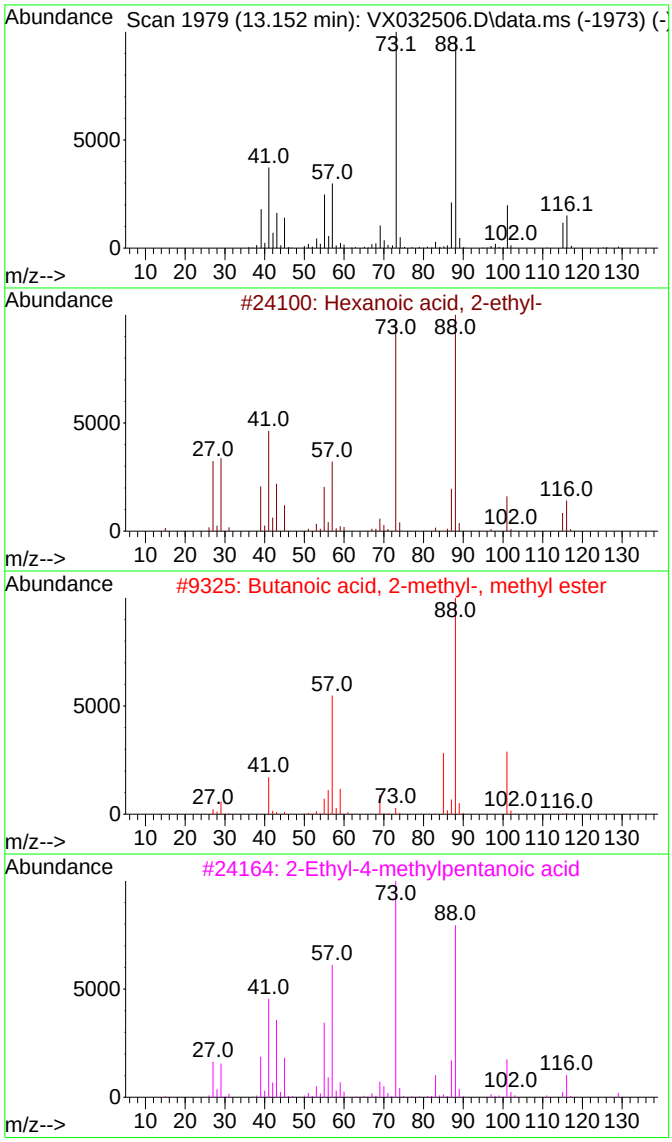
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X102622W.M
Quant Title : SW846 8260

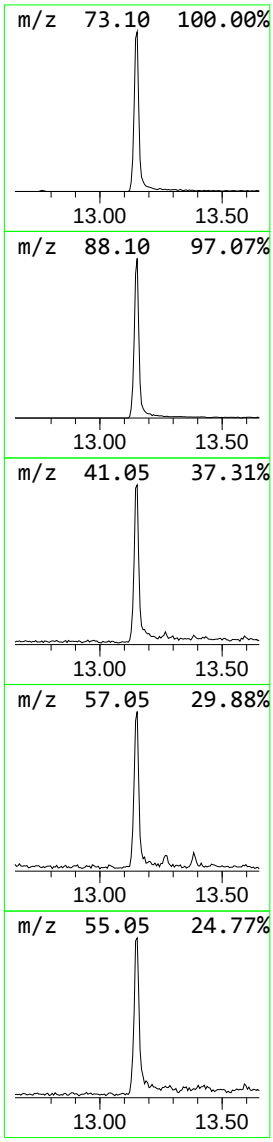
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.152	22.25 ug/l	225774	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Butanoic acid, 2-methyl-, methyl...	116	C6H12O2	000868-57-5	50
3	2-Ethyl-4-methylpentanoic acid	144	C8H16O2	000108-81-6	50
4	Heptanoic acid, 2-ethyl-	158	C9H18O2	003274-29-1	42
5	Methyl 2,3,4-tri-O-methyl-6-deox...	220	C10H20O5	072983-16-5	40





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Instrument :
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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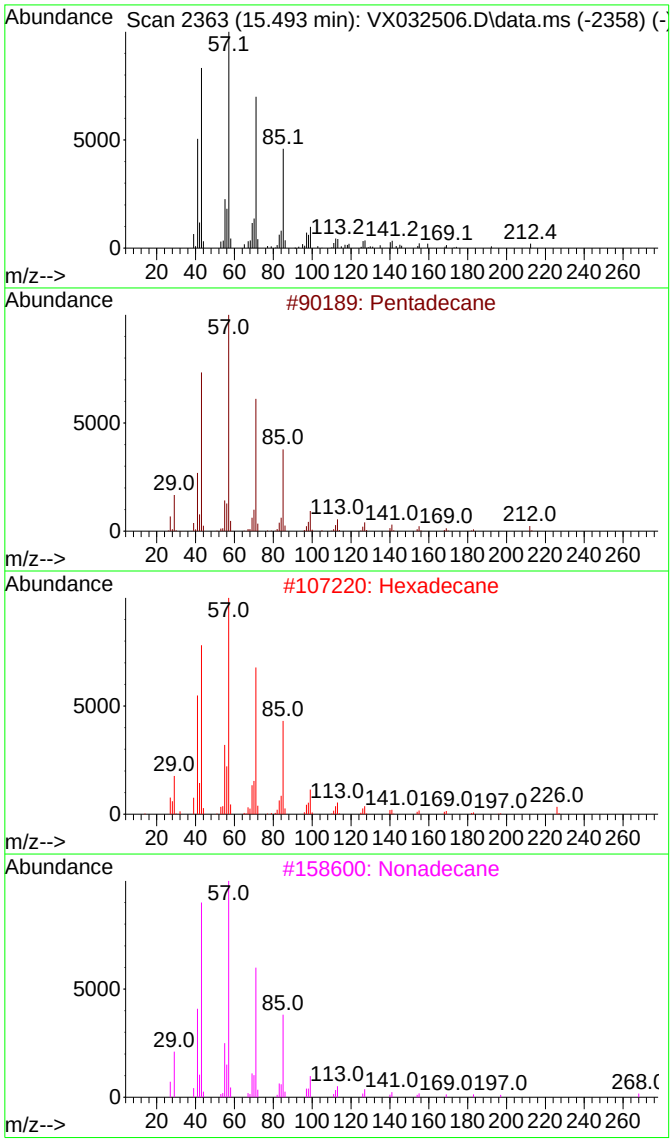
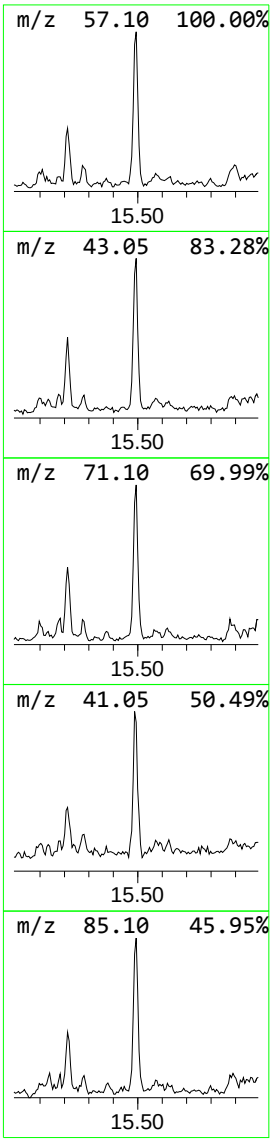
****

Peak Number 6 Pentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.493	6.02 ug/l	61085	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	94
2	Hexadecane	226	C16H34	000544-76-3	91
3	Nonadecane	268	C19H40	000629-92-5	91
4	Tridecane	184	C13H28	000629-50-5	91
5	Tetradecane	198	C14H30	000629-59-4	91





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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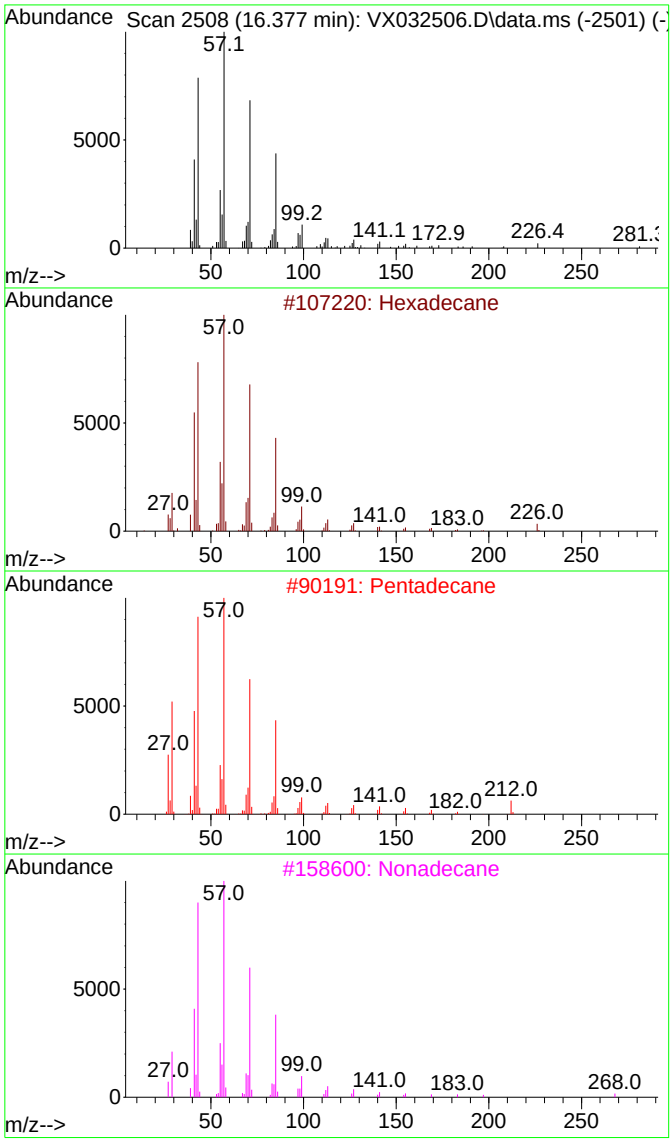
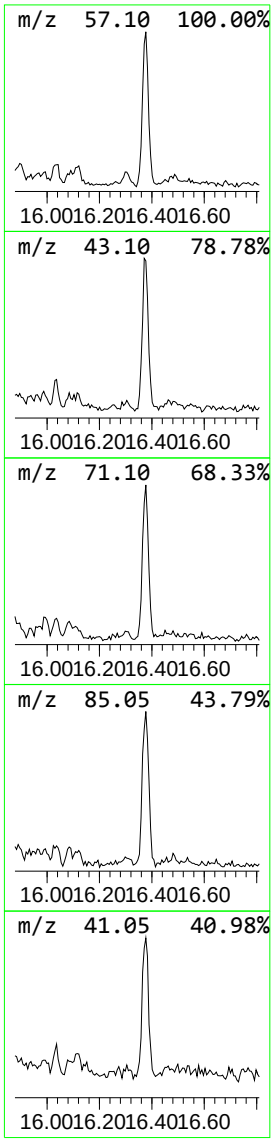
****

Peak Number 7 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.377	6.88 ug/l	69780	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	97
2	Pentadecane	212	C15H32	000629-62-9	91
3	Nonadecane	268	C19H40	000629-92-5	91
4	Tetradecane	198	C14H30	000629-59-4	91
5	Tridecane	184	C13H28	000629-50-5	91





Tentatively Identified Compound (LSC) summary

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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
Ethanol	2.099	55.1	ug/l	398154	1	5.556	361588	50.0
Isopropyl Alcohol	2.557	10.0	ug/l	72004	1	5.556	361588	50.0
1-Hexanol, 2-et...	12.219	42.6	ug/l	432587	4	12.024	507293	50.0
Hexanoic acid, ...	13.152	22.3	ug/l	225774	4	12.024	507293	50.0
Pentadecane	15.493	6.0	ug/l	61085	4	12.024	507293	50.0
Hexadecane	16.377	6.9	ug/l	69780	4	12.024	507293	50.0