LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039604.D
Acq On : 03 Jan 2024 15:59
Operator : JC/MD
Sample : P1002-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1216

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\82X121323W.M
Title : SW846 8260

Signal : TIC: VX039604.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	21	rVB	278876	292155	1.76%	0.612%
2	1.252	24	27	41	rVV	13650643	16577559	100.00%	34.703%
3	1.355	41	44	53	rVV2	179524	231925	1.40%	0.486%
4	1.453	56	60	72	rVB	1641151	2101620	12.68%	4.400%
5	2.050	151	158	172	rBV	636686	1051508	6.34%	2.201%
6	2.374	205	211	229	rBV	920088	1524226	9.19%	3.191%
7	2.947	297	305	317	rBV	72764	166939	1.01%	0.349%
8	4.227	498	515	530	rBV	481516	1303102	7.86%	2.728%
9	4.544	557	567	586	rBV	238711	669233	4.04%	1.401%
10	5.385	693	705	720	rBV2	75870	222451	1.34%	0.466%
11	5.550	723	732	749	rVB	106112	302901	1.83%	0.634%
12	5.952	788	798	806	rBV	84399	227324	1.37%	0.476%
13	6.099	816	822	834	rVB	97360	257127	1.55%	0.538%
14	6.757	922	930	942	rBV	203584	485759	2.93%	1.017%
15	7.196	993	1002	1015	rBV	200651	441438	2.66%	0.924%
16	7.452	1035	1044	1052	rBV	151886	295849	1.78%	0.619%
17	8.647	1234	1240	1246	rBV	441024	699858	4.22%	1.465%
18	8.714	1246	1251	1255	rBV	184099	290102	1.75%	0.607%
19	8.763	1255	1259	1264	rVB	140903	197819	1.19%	0.414%
20	10.055	1461	1471	1476	rBV	510454	784053	4.73%	1.641%
21	10.153	1482	1487	1491	rBV	247254	336545	2.03%	0.705%
22	10.299	1506	1511	1520	rVB	346384	484268	2.92%	1.014%
23	10.500	1539	1544	1550	rVB	242133	306749	1.85%	0.642%
24	10.640	1562	1567	1570	rBV	173312	232958	1.41%	0.488%
25	10.677	1570	1573	1580	rVB	831157	1009057	6.09%	2.112%
26	10.750	1580	1585	1592	rBV3	436158	653556	3.94%	1.368%
27	11.079	1633	1639	1643	rBV	478895	621010	3.75%	1.300%
28	11.128	1643	1647	1652	rVB	432310	512035	3.09%	1.072%
29	11.476	1698	1704	1712	rVB2	111990	166299	1.00%	0.348%
30	11.567	1712	1719	1722	rBV2	317527	502476	3.03%	1.052%
31	11.604	1722	1725	1731	rVV3	243618	388778	2.35%	0.814%
32	11.683	1734	1738	1744	rVB	590883	676804	4.08%	1.417%
33	11.750	1744	1749	1754	rBV2	142197	208379	1.26%	0.436%
34	11.835	1758	1763	1765	rVV2	138449	203221	1.23%	0.425%
35	11.866	1765	1768	1779	rVB3	159983	381758	2.30%	0.799%
36	12.018	1789	1793	1801	rVB2	581875	838625	5.06%	1.756%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039604.D
Acq On : 03 Jan 2024 15:59
Operator : JC/MD
Sample : P1002-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1216

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\82X121323W.M
Title : SW846 8260

37	12.219	1821	1826	1836	rBV	8605392	10494429	63.31%	21.969%
38	12.305	1836	1840	1853	rVB2	279651	471510	2.84%	0.987%
39	12.561	1877	1882	1886	rBV3	156161	208526	1.26%	0.437%
40	13.676	2060	2065	2069	rBV	135182	179375	1.08%	0.376%
41	13.750	2073	2077	2079	rBV	223079	292493	1.76%	0.612%
42	13.774	2079	2081	2085	rVB	262937	288988	1.74%	0.605%
43	13.841	2090	2092	2100	rVV2	126259	188454	1.14%	0.395%

Sum of corrected areas: 47769241

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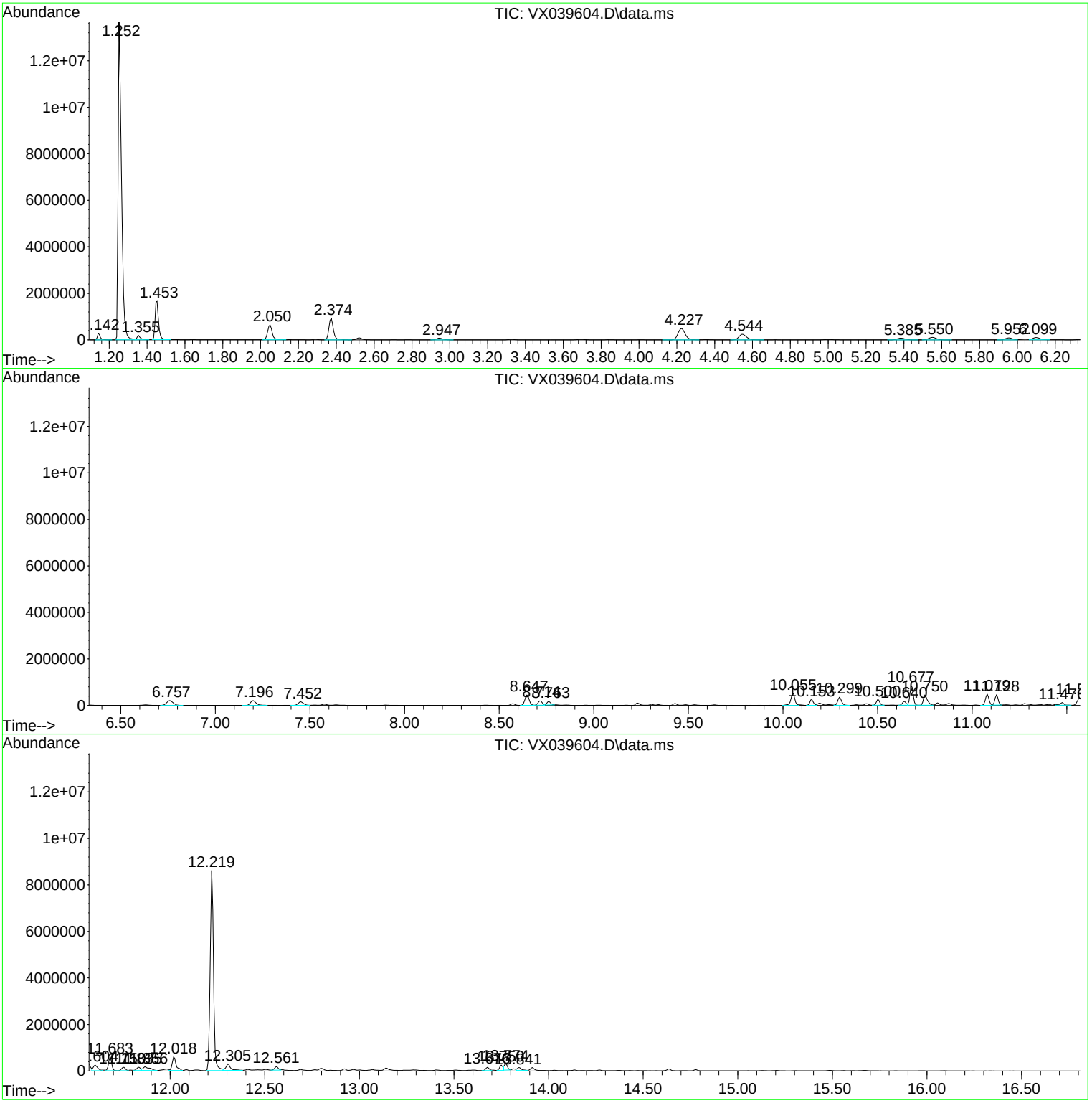
MSVOA_X
ClientSampleId :
1216

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039604.D
Acq On : 03 Jan 2024 15:59
Operator : JC/MD
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
1216

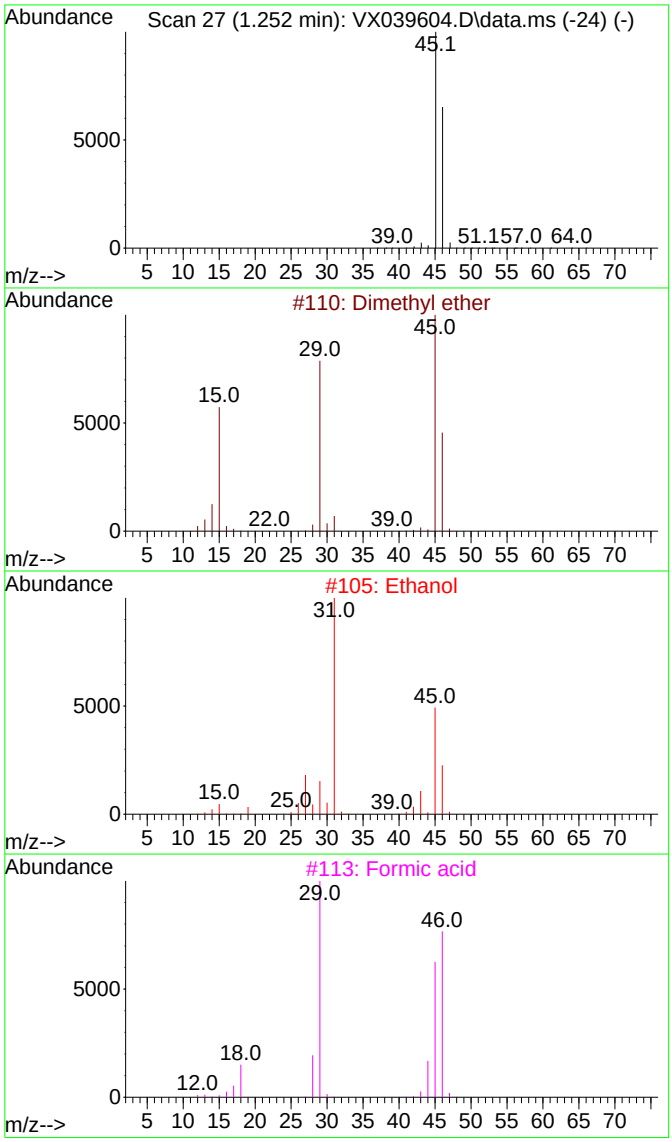
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

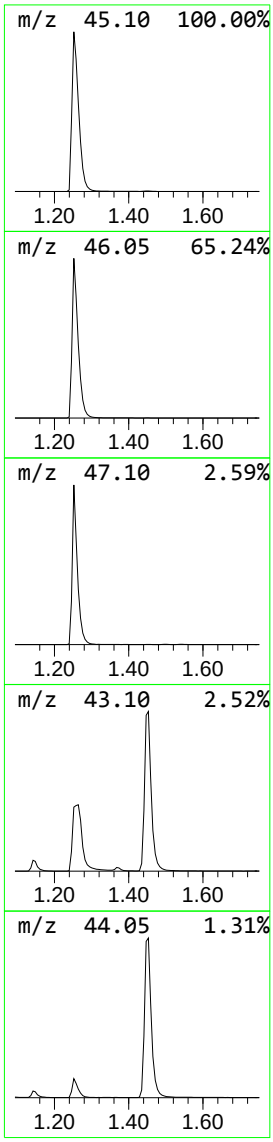
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Dimethyl ether Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	2736.46 ug/l	16577600	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl ether	46	C2H6O	000115-10-6	86
2	Ethanol	46	C2H6O	000064-17-5	7
3	Formic acid	46	CH2O2	000064-18-6	7
4	Ethene, fluoro-	46	C2H3F	000075-02-5	4
5	Hydrazine, methyl-	46	CH6N2	000060-34-4	4





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Data File : VX039604.D
Acq On : 03 Jan 2024 15:59
Operator : JC/MD
Sample : P1002-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1216

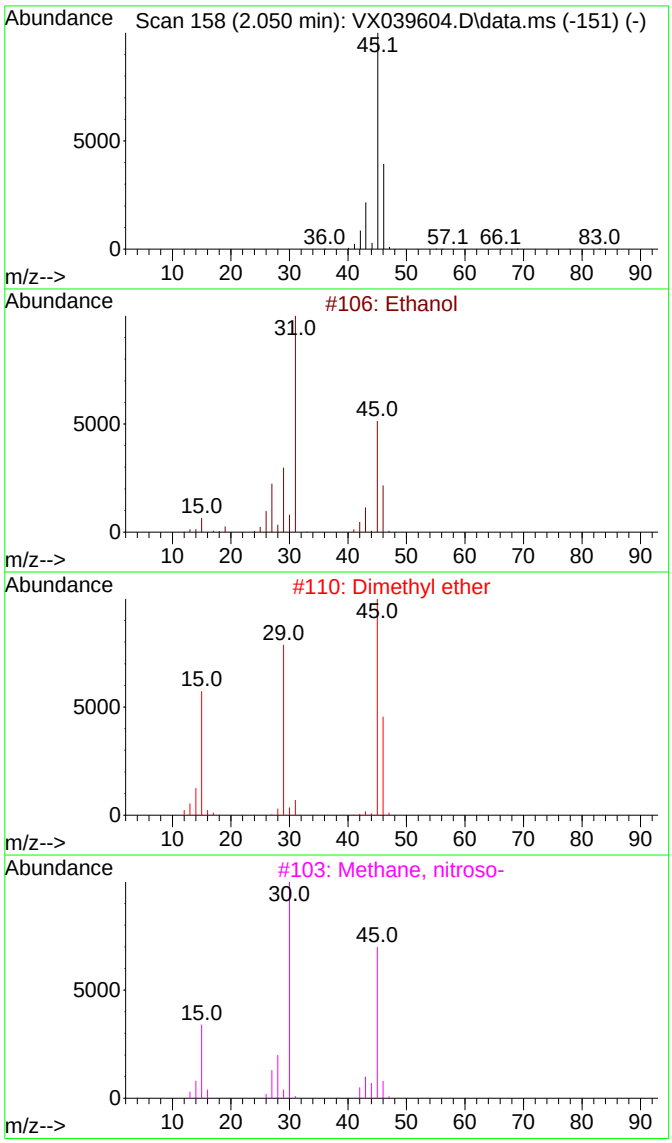
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

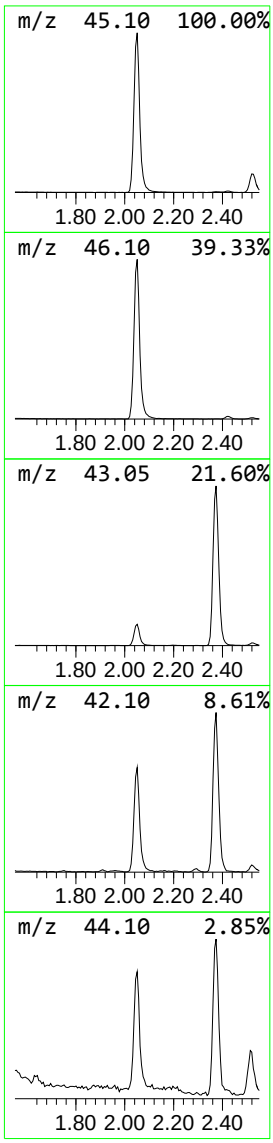
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.050	173.57 ug/l	1051510	Pentafluorobenzene	5.550

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039604.D
Acq On : 03 Jan 2024 15:59
Operator : JC/MD
Sample : P1002-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1216

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

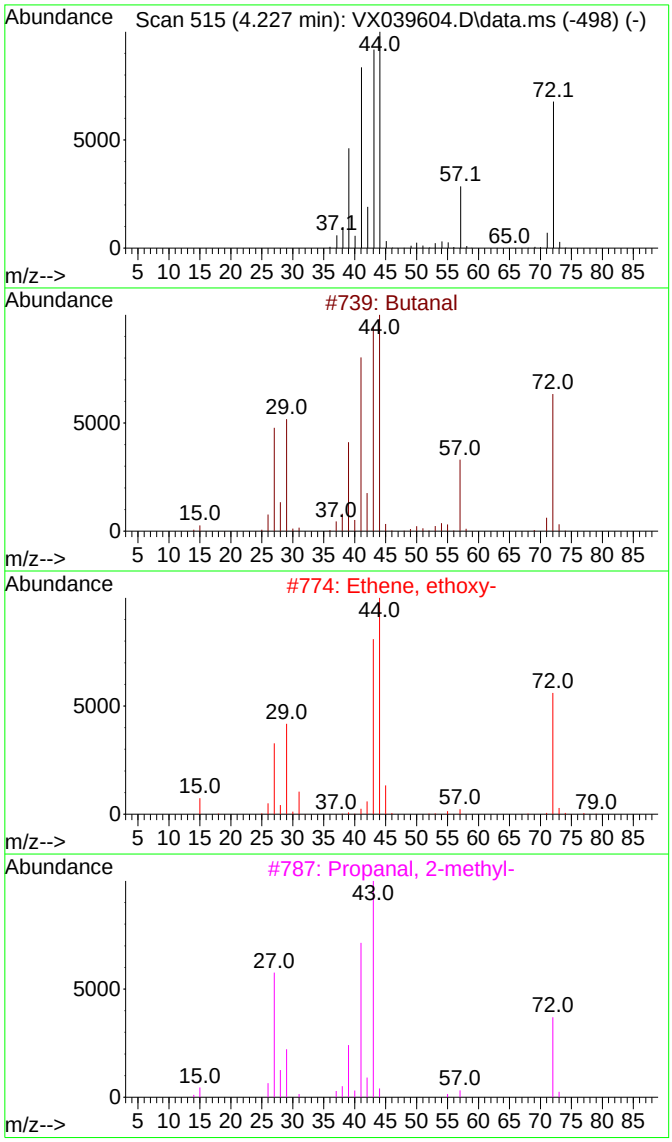
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

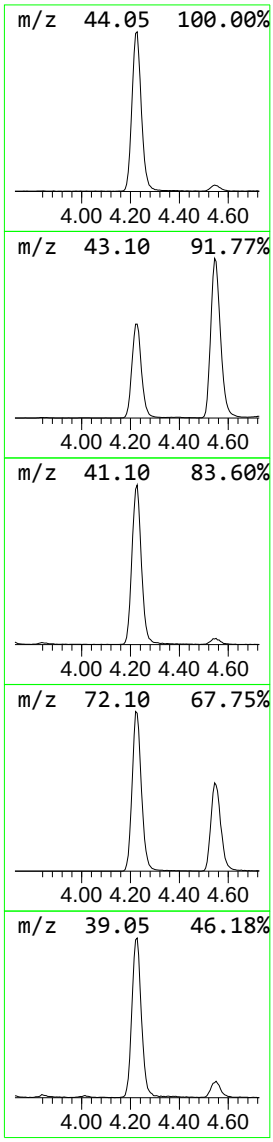
****

Peak Number 5 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	215.10 ug/l	1303100	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	49
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
4	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	27
5	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	23





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039604.D
Acq On : 03 Jan 2024 15:59
Operator : JC/MD
Sample : P1002-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1216

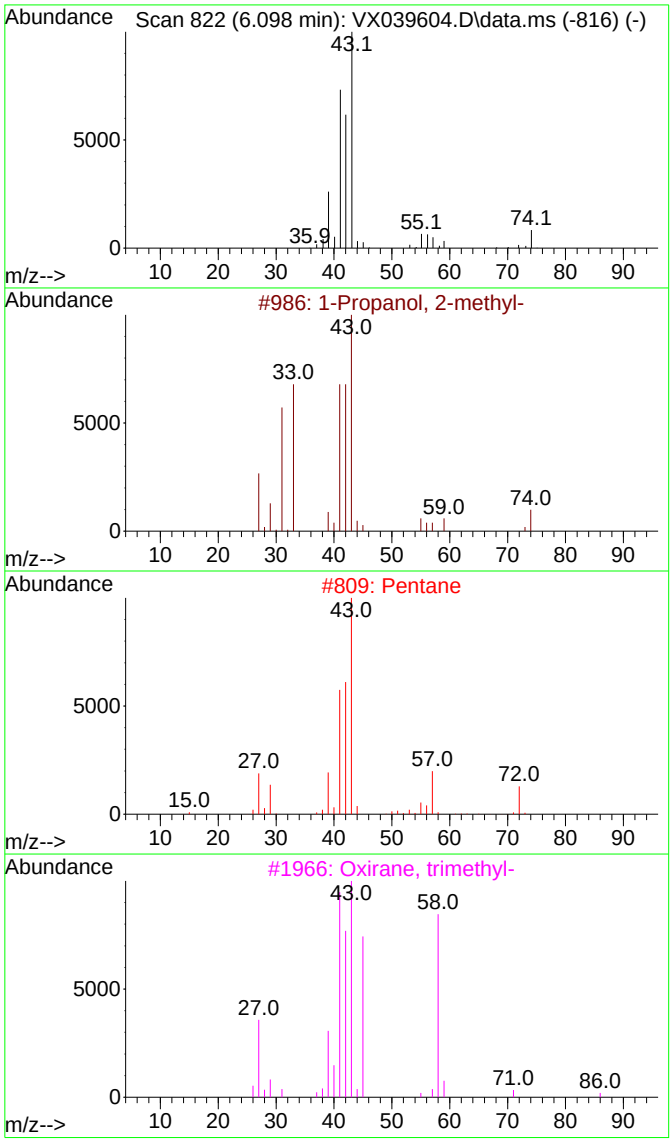
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

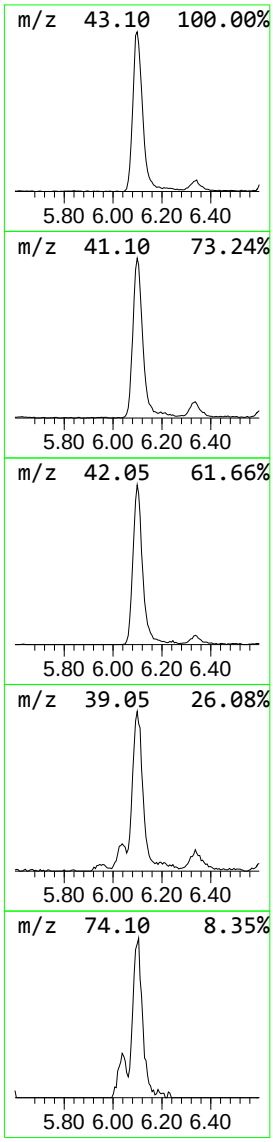
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Propanol, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.098	42.44 ug/l	257127	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	78
2	Pentane	72	C5H12	000109-66-0	40
3	Oxirane, trimethyl-	86	C5H10O	005076-19-7	39
4	Isobutylene epoxide	72	C4H8O	000558-30-5	33
5	Propanal, 2-methyl-	72	C4H8O	000078-84-2	27





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Acq On : 03 Jan 2024 15:59
Operator : JC/MD
Sample : P1002-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1216

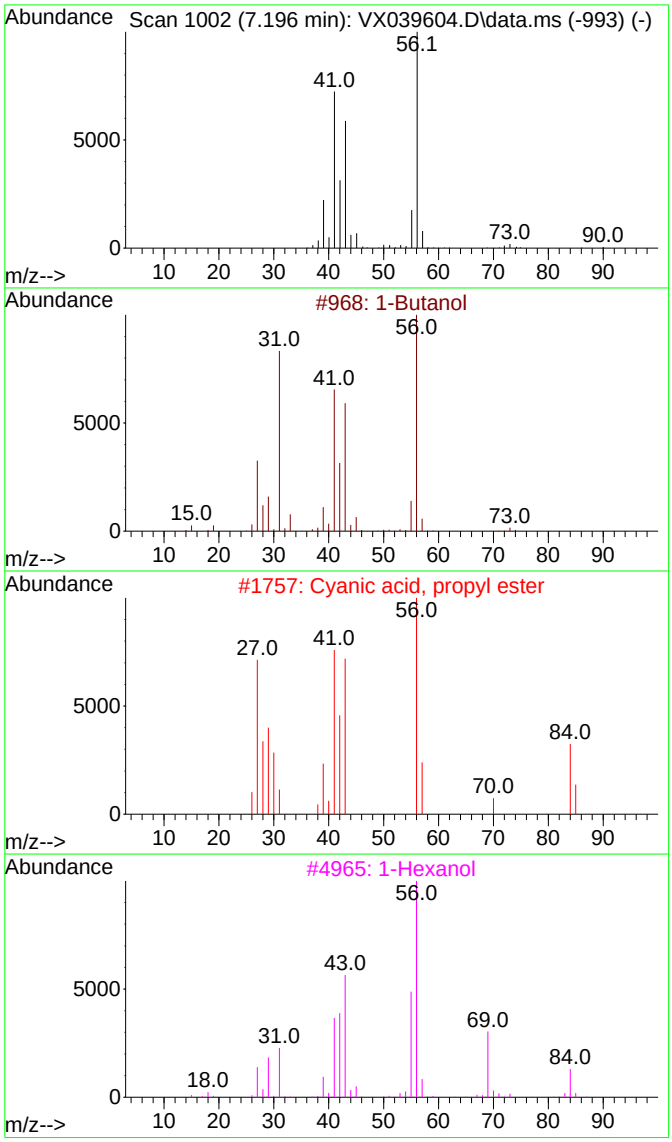
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

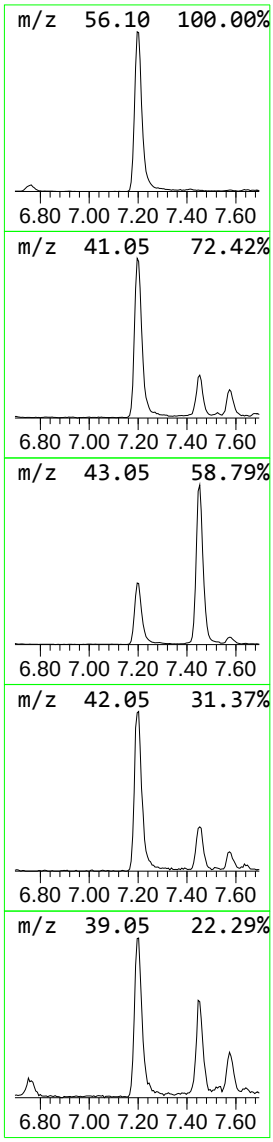
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1-Butanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.196	45.44 ug/l	441438	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	90
2	Cyanic acid, propyl ester	85	C4H7NO	001768-36-1	50
3	1-Hexanol	102	C6H14O	000111-27-3	43
4	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	38
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	36





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Data File : VX039604.D
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1216

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

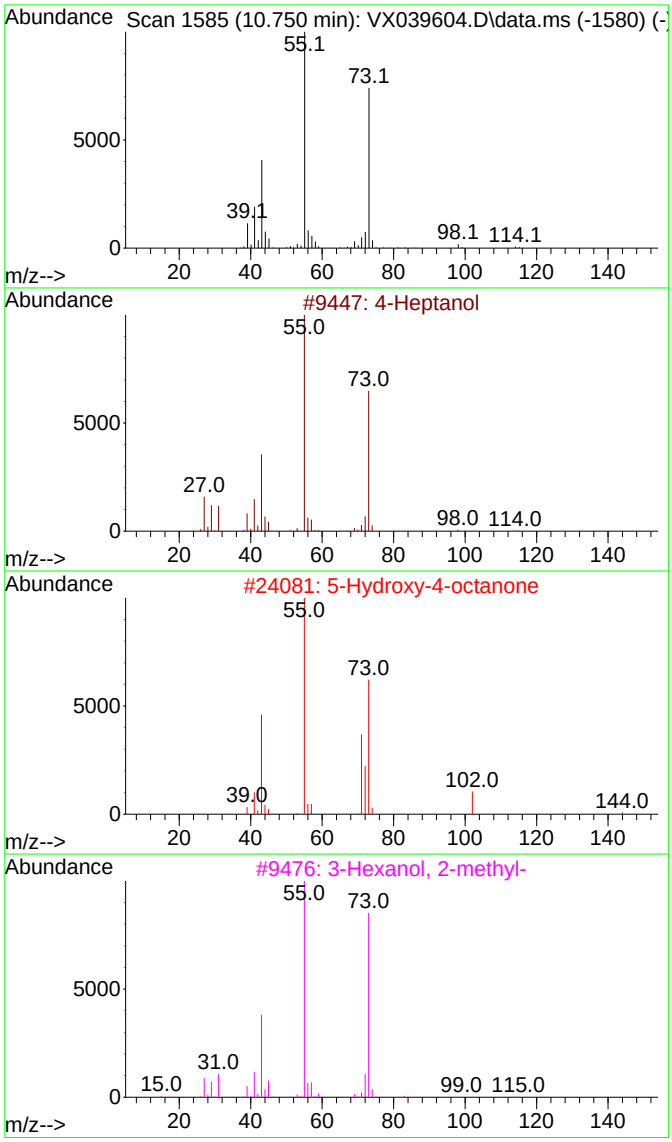
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

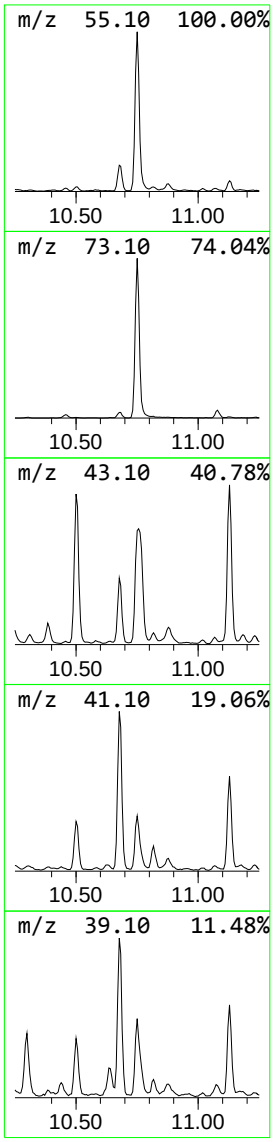
****

Peak Number 8 4-Heptanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.750	41.68 ug/l	653556	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol	116	C7H16O	000589-55-9	78
2	5-Hydroxy-4-octanone	144	C8H16O2	000496-77-5	64
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	50
4	4,5-Octanediol	146	C8H18O2	022607-10-9	38
5	3,5-Dimethyl-5-hexen-3-ol	128	C8H16O	001569-46-6	23





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1216

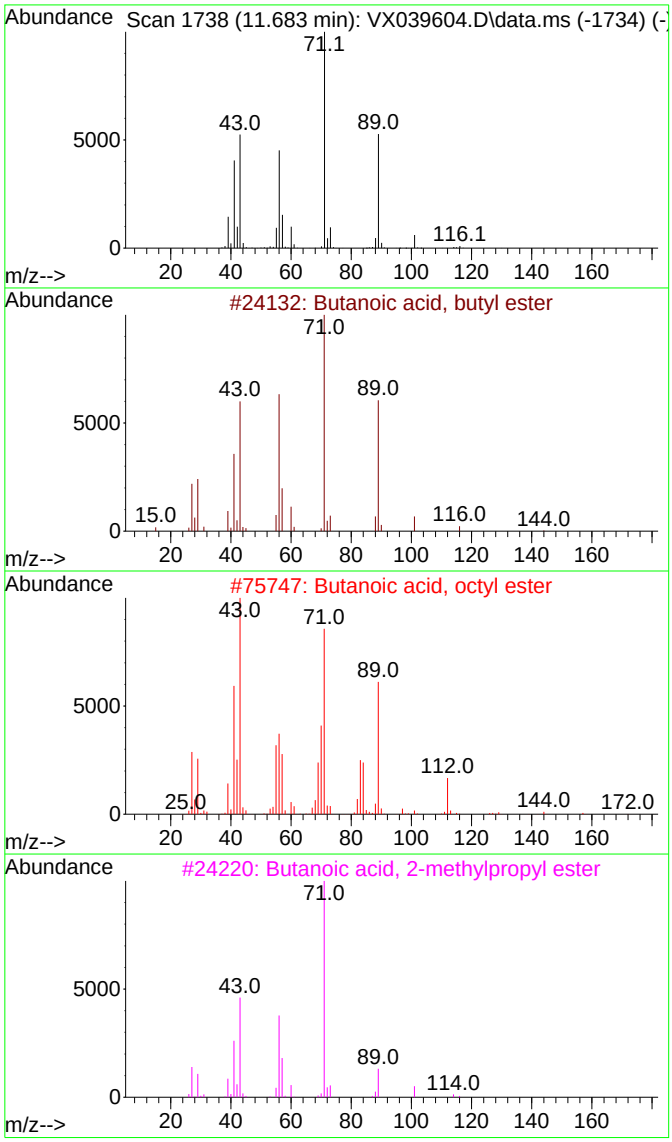
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

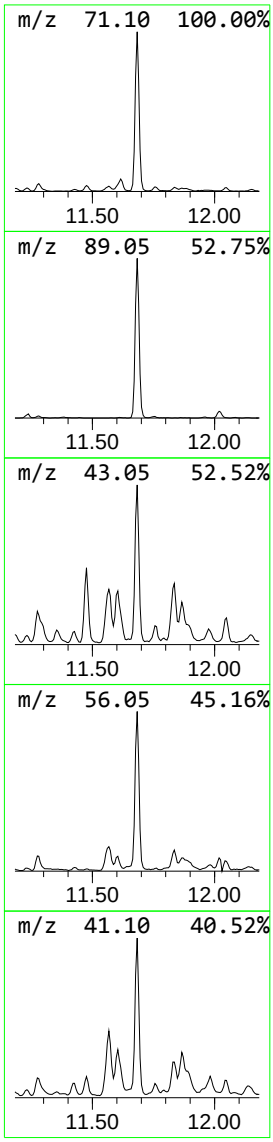
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Butanoic acid, butyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	40.35 ug/l	676804	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
3	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	72
5	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	56





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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1216

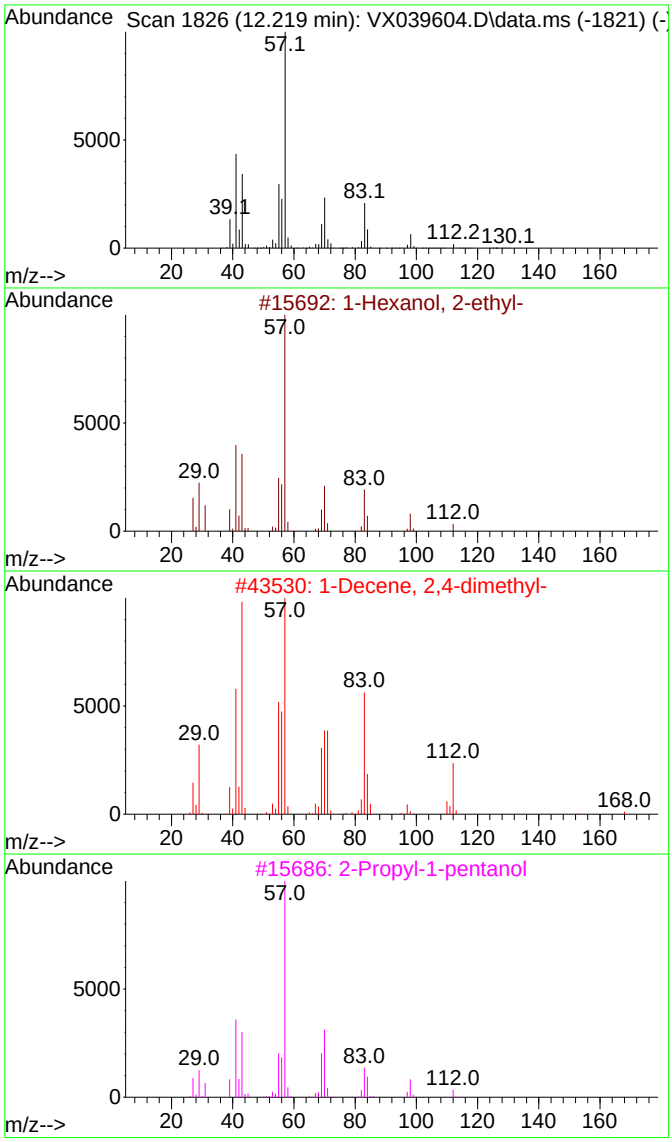
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

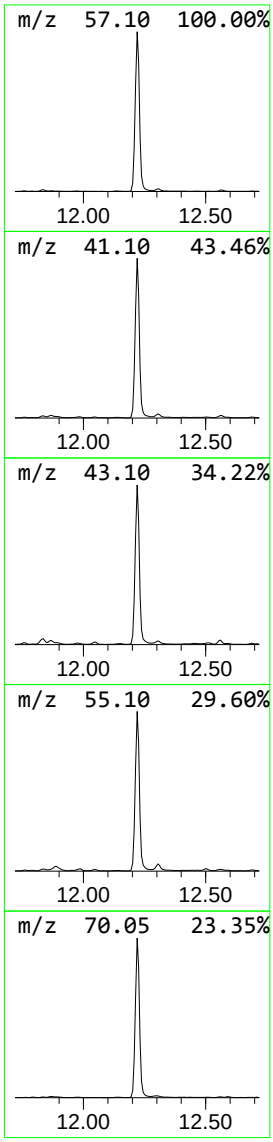
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	625.69 ug/l	10494400	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	50
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	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039604.D
Acq On : 03 Jan 2024 15:59
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1216

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
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
Dimethyl ether	1.252	2736.5	ug/l	16577600	1	5.550	302901	50.0
Ethanol	2.050	173.6	ug/l	1051510	1	5.550	302901	50.0
Butanal	4.227	215.1	ug/l	1303100	1	5.550	302901	50.0
1-Propanol, 2-m...	6.098	42.4	ug/l	257127	1	5.550	302901	50.0
1-Butanol	7.196	45.4	ug/l	441438	2	6.757	485759	50.0
4-Heptanol	10.750	41.7	ug/l	653556	3	10.055	784053	50.0
Butanoic acid, ...	11.683	40.4	ug/l	676804	4	12.018	838625	50.0
1-Hexanol, 2-et...	12.219	625.7	ug/l	10494400	4	12.018	838625	50.0