LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021524\
Data File : VX040248.D
Acq On : 15 Feb 2024 13:42
Operator : JC/MD
Sample : P1424-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1285

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\82X020924W.M
Title : SW846 8260

Signal : TIC: VX040248.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.148	6	10	18	rVB	35627	40146	6.02%	0.933%
2	1.368	41	46	54	rBV2	4586	7887	1.18%	0.183%
3	1.453	56	60	68	rVB	6246	6937	1.04%	0.161%
4	2.050	152	158	167	rBV	17241	28847	4.33%	0.670%
5	2.380	206	212	223	rBV	16679	28129	4.22%	0.654%
6	2.526	228	236	247	rBV	6278	12477	1.87%	0.290%
7	2.703	258	265	275	rVB2	4110	8174	1.23%	0.190%
8	2.947	299	305	316	rVB3	3067	6997	1.05%	0.163%
9	4.227	506	515	531	rBV2	28030	77065	11.56%	1.791%
10	4.568	563	571	586	rBV	3706	11205	1.68%	0.260%
11	5.385	694	705	719	rBV	48851	140554	21.08%	3.267%
12	5.550	722	732	746	rVV	79142	223610	33.53%	5.197%
13	5.958	788	799	809	rBV	54687	141936	21.28%	3.299%
14	6.757	921	930	942	rBV	127680	302183	45.31%	7.023%
15	7.214	997	1005	1017	rBV3	11420	33698	5.05%	0.783%
16	8.647	1234	1240	1248	rBV	274596	419115	62.85%	9.740%
17	10.055	1462	1471	1482	rBV	279740	398748	59.79%	9.267%
18	10.159	1482	1488	1498	rBV4	7519	18139	2.72%	0.422%
19	10.305	1507	1512	1518	rVB4	3747	6754	1.01%	0.157%
20	10.506	1541	1545	1555	rVB	9477	13877	2.08%	0.323%
21	10.683	1570	1574	1580	rVB	15903	19957	2.99%	0.464%
22	10.750	1580	1585	1595	rBV	80625	132027	19.80%	3.068%
23	11.079	1633	1639	1644	rBV	251447	317239	47.57%	7.373%
24	11.128	1644	1647	1654	rVB	19264	26498	3.97%	0.616%
25	11.232	1661	1664	1668	rBV2	5362	6989	1.05%	0.162%
26	11.280	1668	1672	1675	rBV	8012	10484	1.57%	0.244%
27	11.390	1686	1690	1692	rBV3	5124	7314	1.10%	0.170%
28	11.421	1692	1695	1699	rVB2	7252	9832	1.47%	0.228%
29	11.573	1712	1720	1723	rBV	34678	50117	7.52%	1.165%
30	11.604	1723	1725	1733	rVV	34437	51756	7.76%	1.203%
31	11.683	1733	1738	1747	rVB	595124	666891	100.00%	15.499%
32	11.988	1779	1788	1789	rBV3	16943	34116	5.12%	0.793%
33	12.018	1789	1793	1801	rVB	341332	431293	64.67%	10.023%
34	12.219	1821	1826	1839	rBV	337384	526688	78.98%	12.240%
35	13.603	2045	2053	2061	rBV9	6979	15555	2.33%	0.362%
36	13.676	2061	2065	2070	rVV	32642	40608	6.09%	0.944%

LSC Area Percent Report

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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1285

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\82X020924W.M
Title : SW846 8260

37	14.030	2119	2123	2128	rVB	8371	9678	1.45%	0.225%
38	14.140	2136	2141	2151	rBV2	7453	10665	1.60%	0.248%
39	14.268	2159	2162	2167	rBV2	7467	8687	1.30%	0.202%

Sum of corrected areas: 4302872

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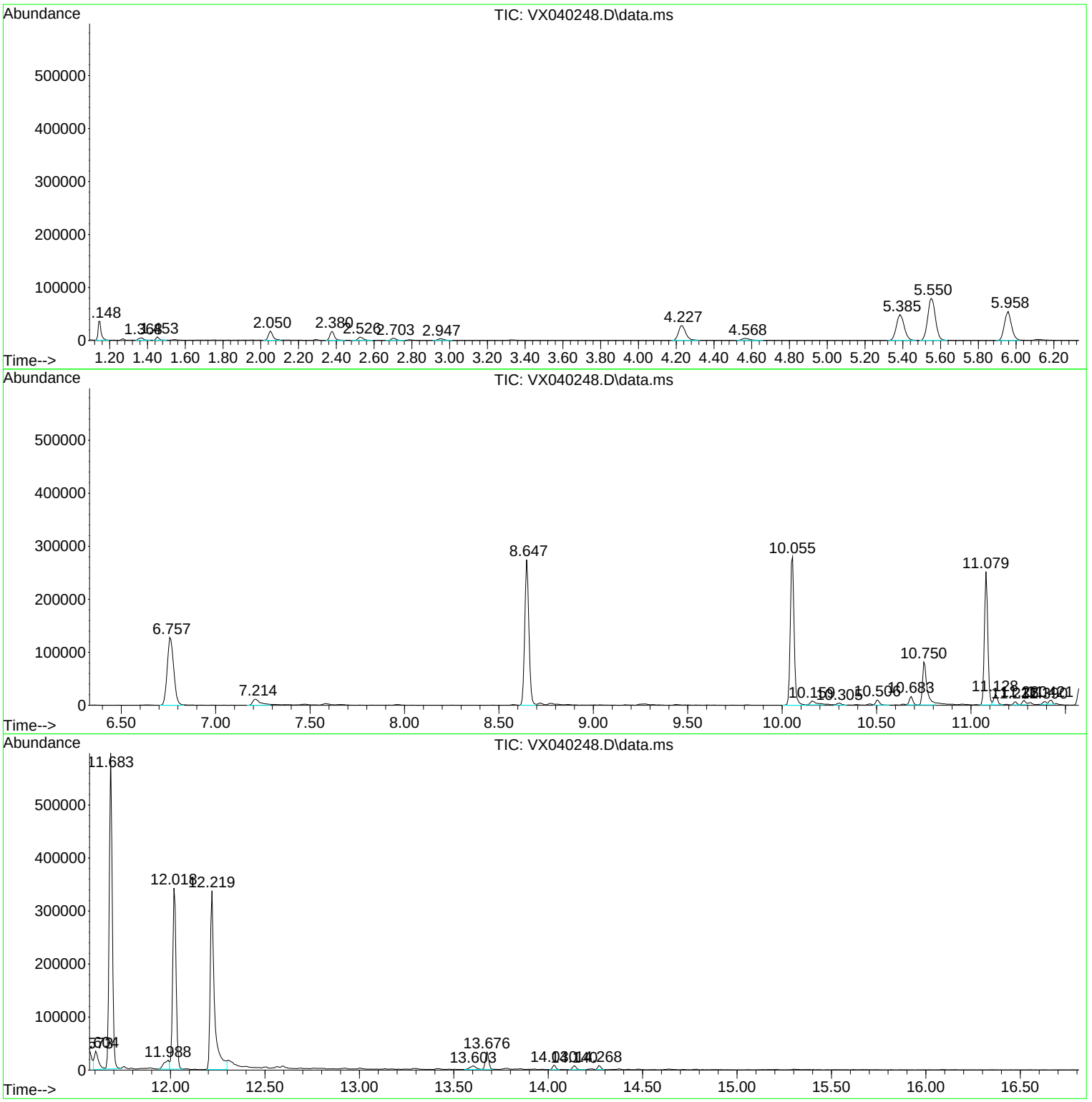
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

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



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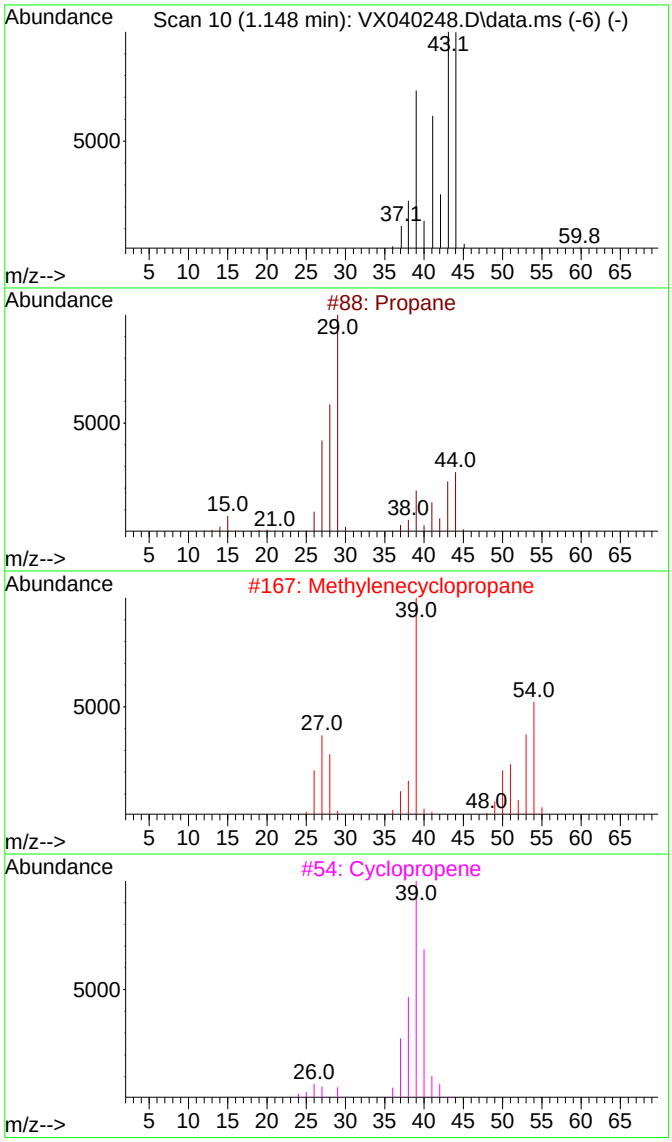
Quant Title : SW846 8260

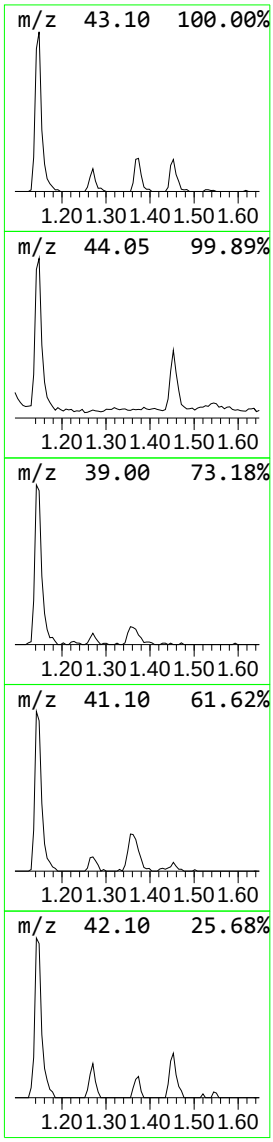
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Propane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.148	8.98 ug/l	40146	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	90
2	Methylenecyclopropane	54	C4H6	006142-73-0	2
3	Cyclopropene	40	C3H4	002781-85-3	2
4	Propene	42	C3H6	000115-07-1	2
5	2-Isopropoxyethylamine	103	C5H13NO	081731-43-3	2





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Operator : JC/MD
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Instrument :
MSVOA_X
ClientSampleId :
1285

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

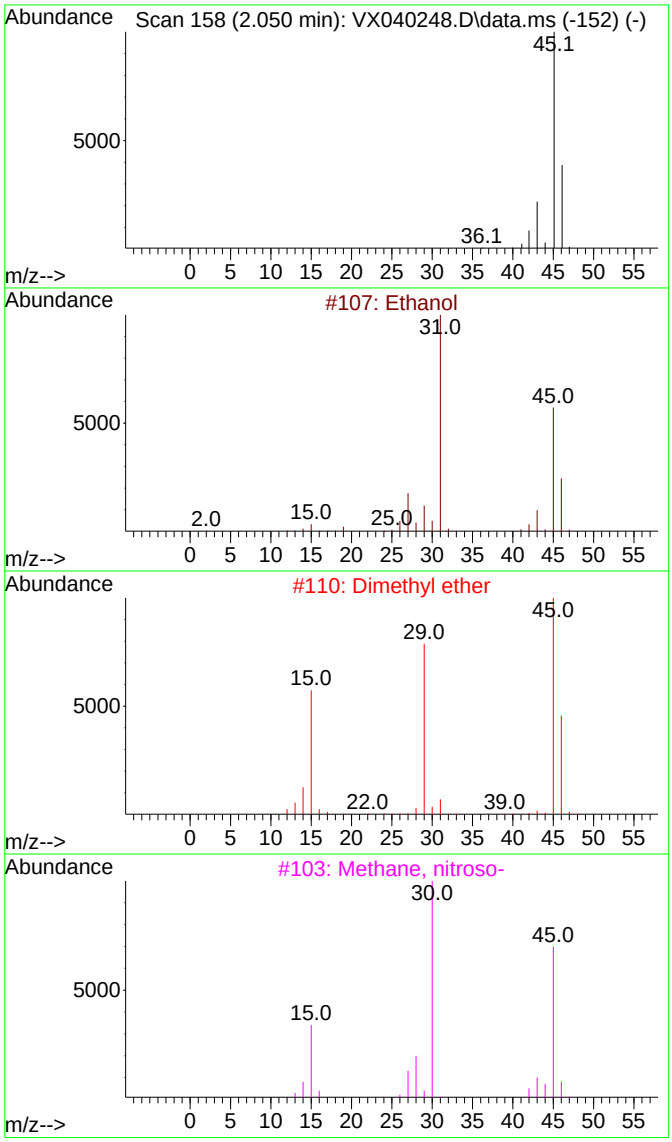
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

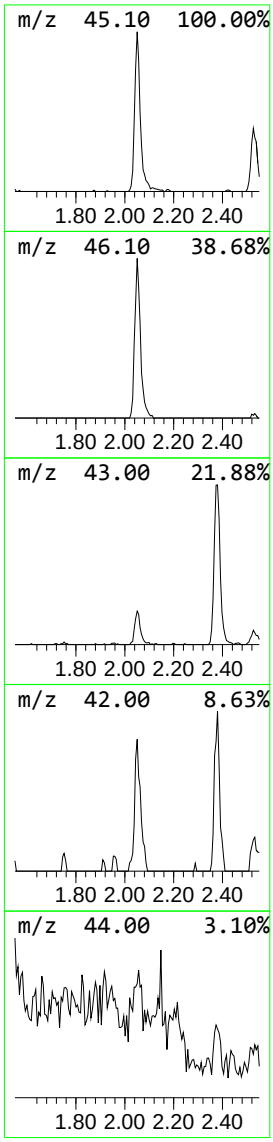
****

Peak Number 2 Ethanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.050	6.45 ug/l	28847	Pentafluorobenzene	5.550

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	L-Lactic acid	90	C3H6O3	000079-33-4	2





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Data File : VX040248.D
Acq On : 15 Feb 2024 13:42
Operator : JC/MD
Sample : P1424-02
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1285

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

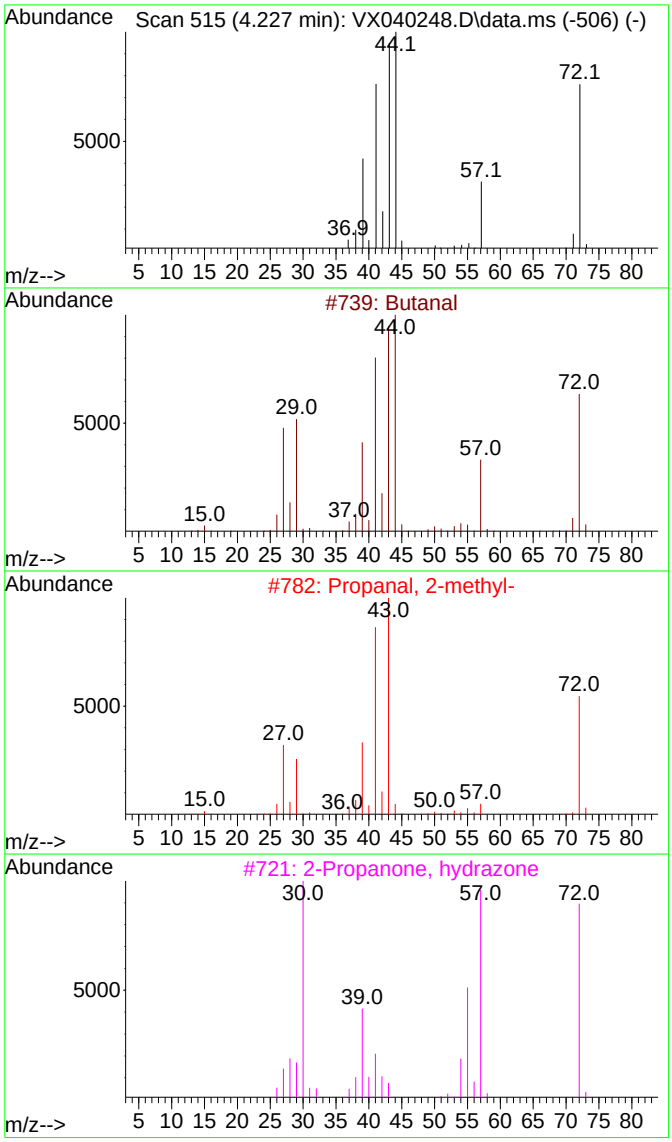
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

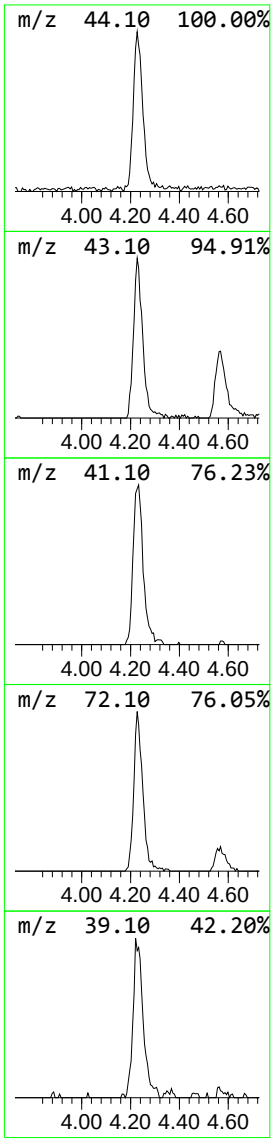
****

Peak Number 3 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	17.23 ug/l	77065	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	43
4	Ethene, ethoxy-	72	C4H8O	000109-92-2	40
5	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37





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Data File : VX040248.D
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Operator : JC/MD
Sample : P1424-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1285

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

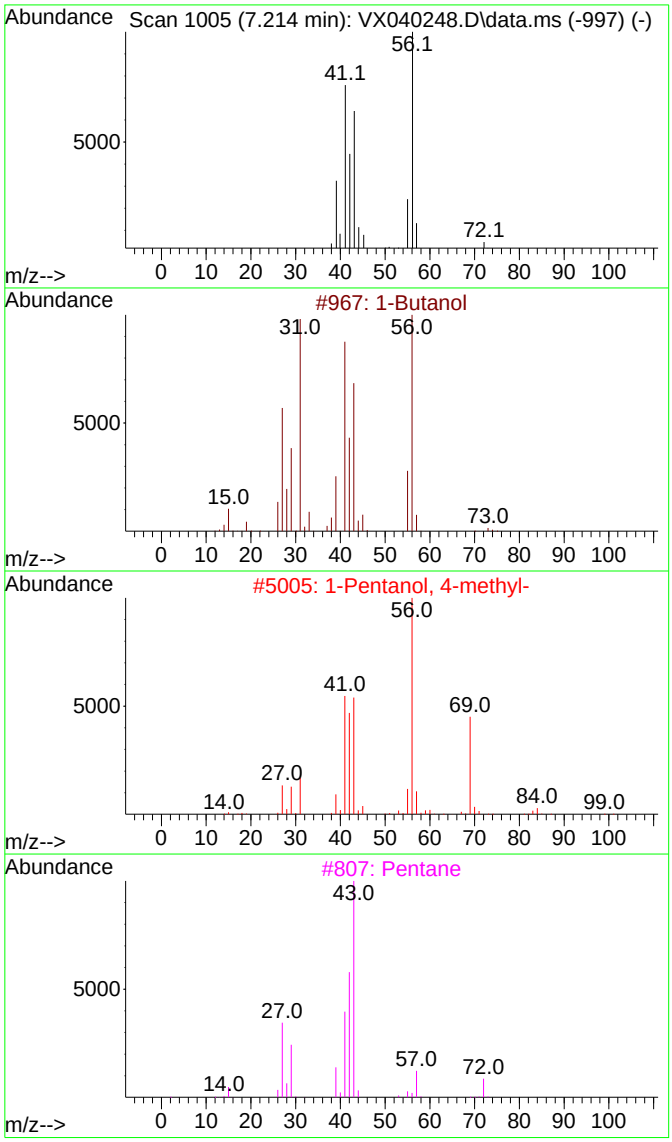
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

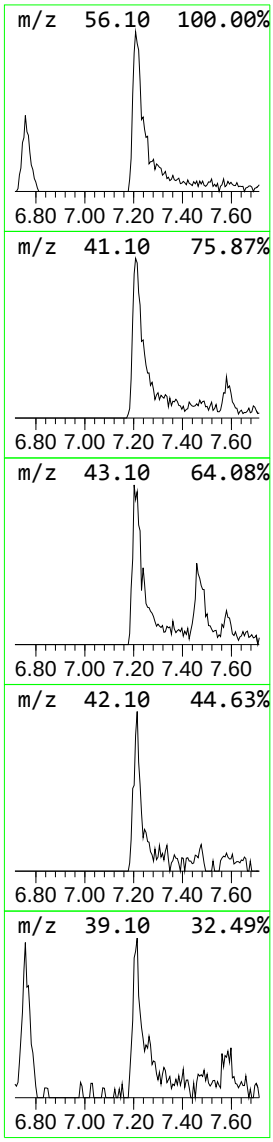
****

Peak Number 4 1-Butanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.214	5.58 ug/l	33698	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	64
2	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	56
3	Pentane	72	C5H12	000109-66-0	9
4	Oxirane, 2-methyl-3-(1-methyleth...	100	C6H12O	001192-31-0	9
5	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9





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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1285

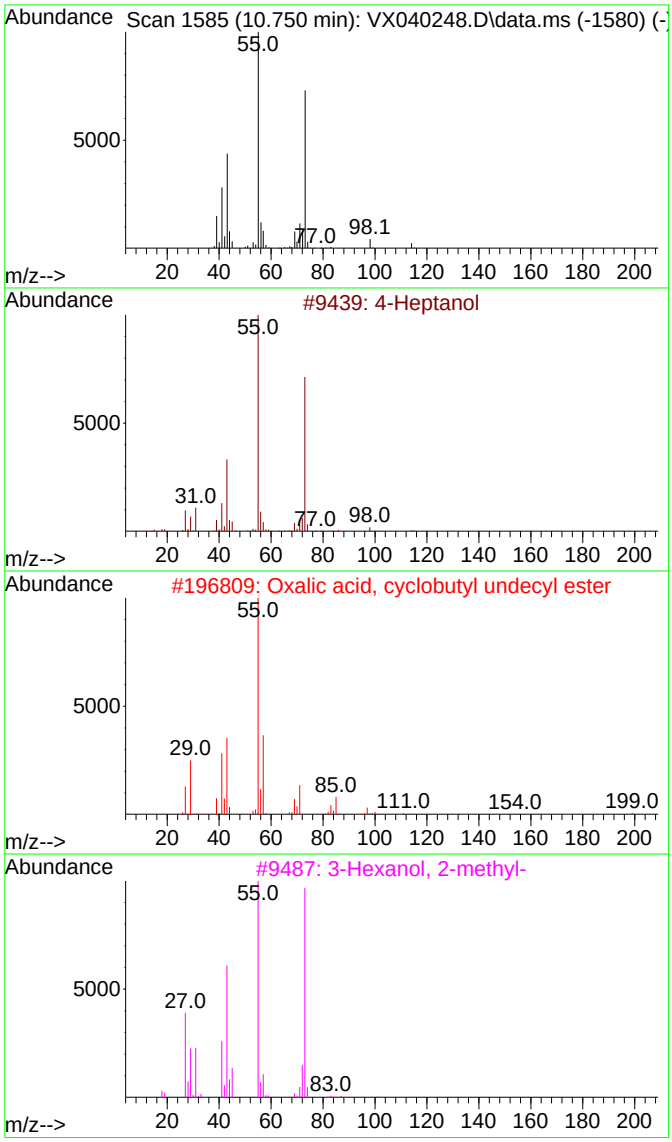
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

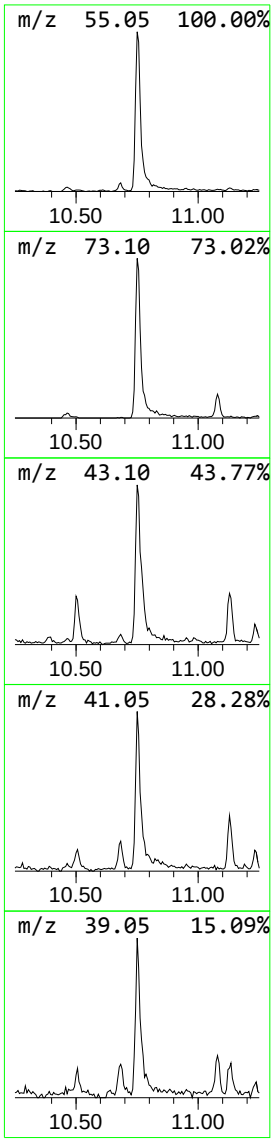
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 4-Heptanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.750	16.56 ug/l	132027	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol	116	C7H16O	000589-55-9	64
2	Oxalic acid, cyclobutyl undecyl ...	298	C17H30O4	1000309-70-2	50
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	50
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	50
5	1-Hepten-4-ol	114	C7H14O	003521-91-3	40





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Instrument :
MSVOA_X
ClientSampleId :
1285

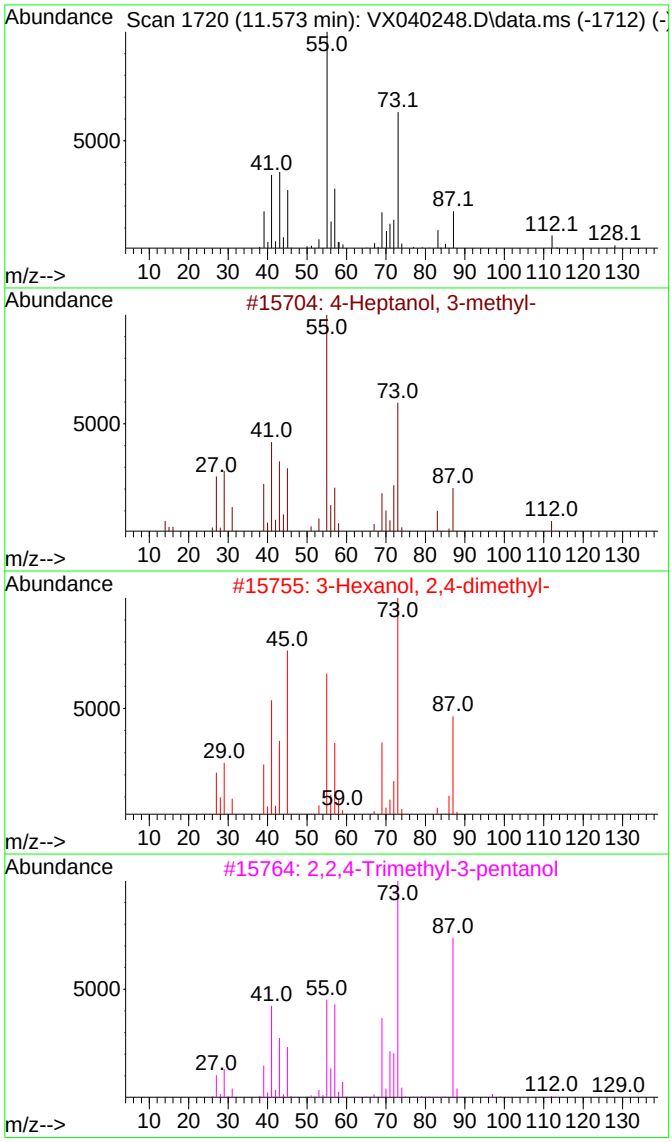
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

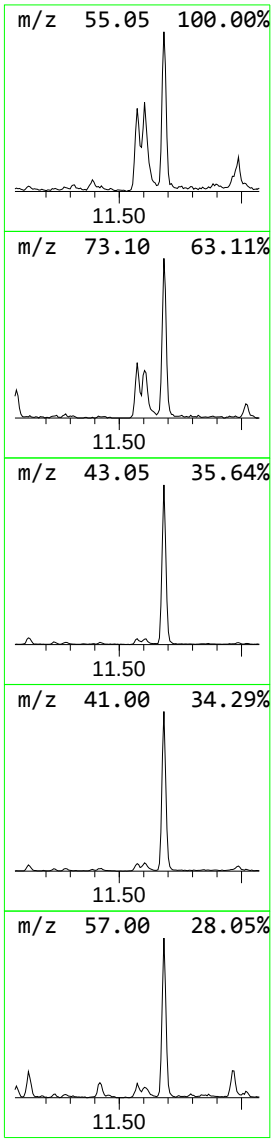
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 4-Heptanol, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.573	5.81 ug/l	50117	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 3-methyl-	130	C8H18O	001838-73-9	64
2	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	47
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	45
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	42
5	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	37





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Instrument :
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ClientSampleId :
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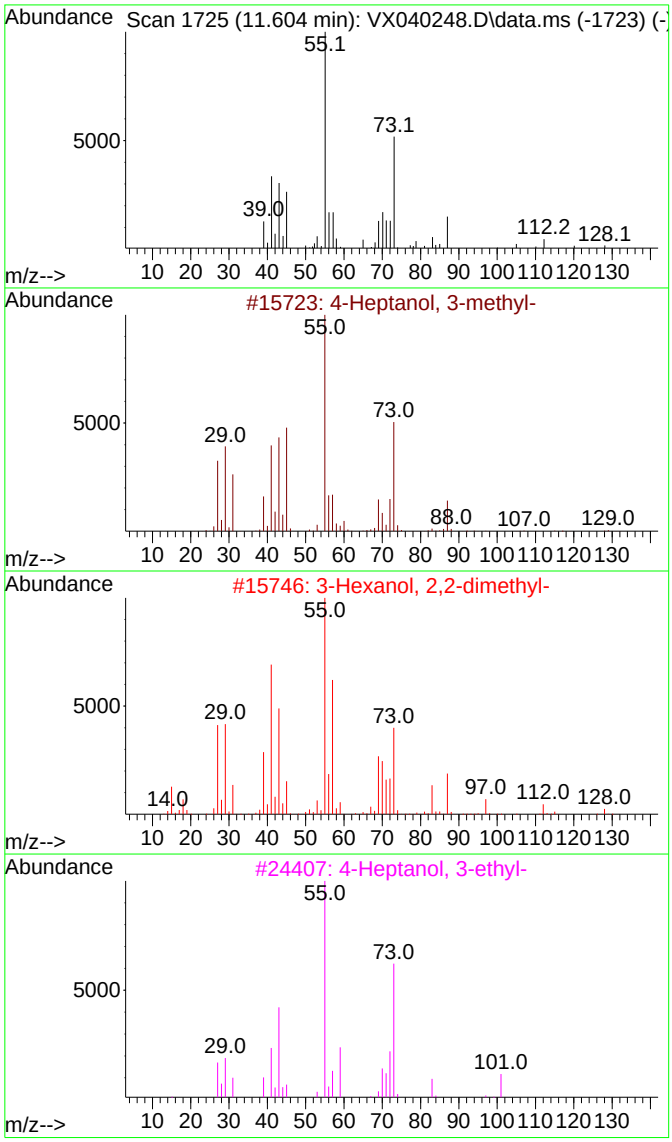
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

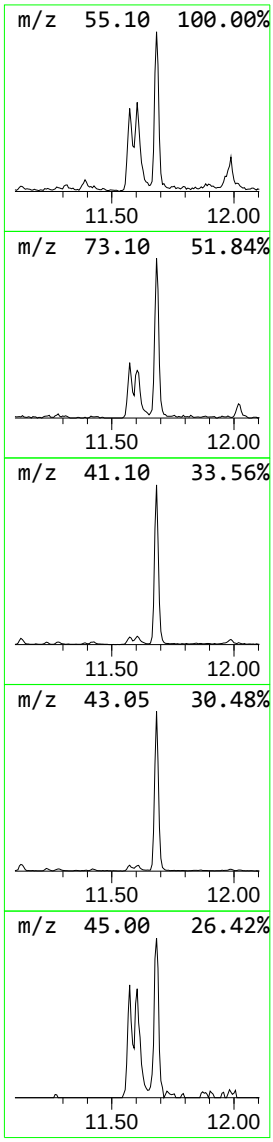
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 3-Hexanol, 2,2-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.604	6.00 ug/l	51756	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 3-methyl-	130	C8H18O	001838-73-9	59
2	3-Hexanol, 2,2-dimethyl-	130	C8H18O	004209-90-9	50
3	4-Heptanol, 3-ethyl-	144	C9H20O	019780-42-8	43
4	Pentanoic acid, 2-(aminooxy)-	133	C5H11NO3	005699-55-8	42
5	1-Butene, 3-(2-butenyloxy)-	126	C8H14O	001476-05-7	25





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MSVOA_X
ClientSampleId :
1285

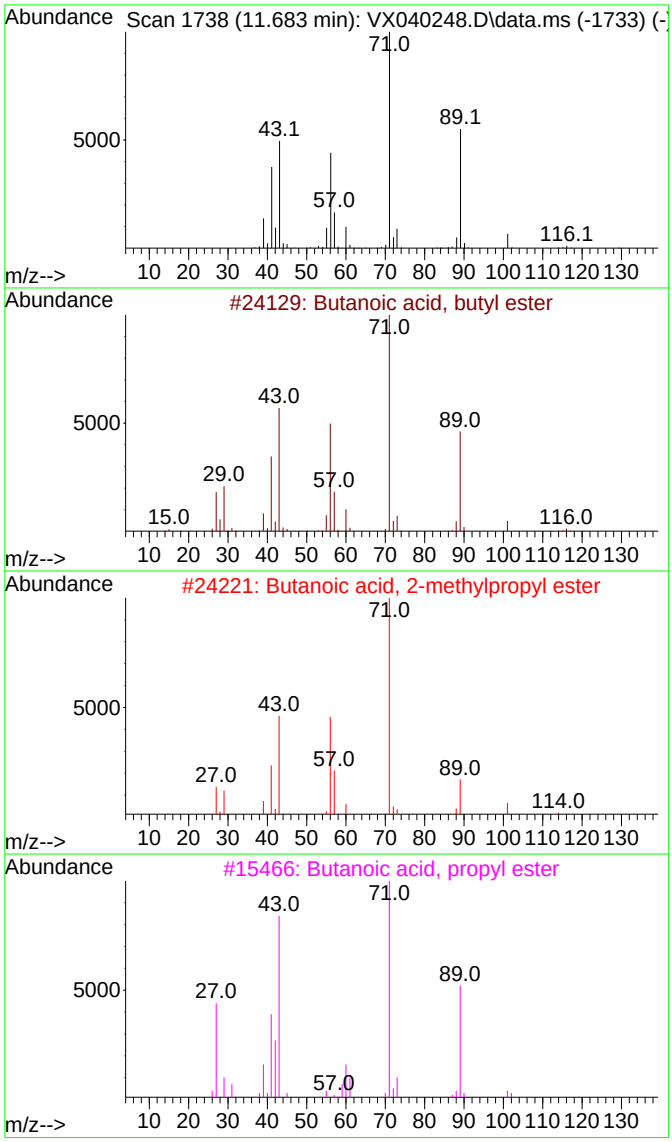
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

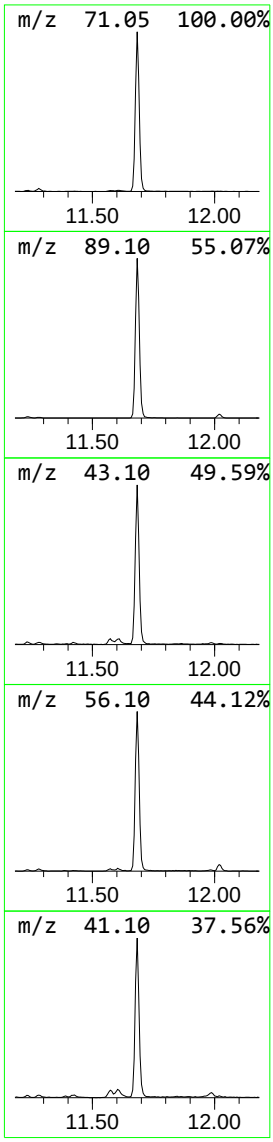
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	77.31 ug/l	666891	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, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	56
5	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	53





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MSVOA_X
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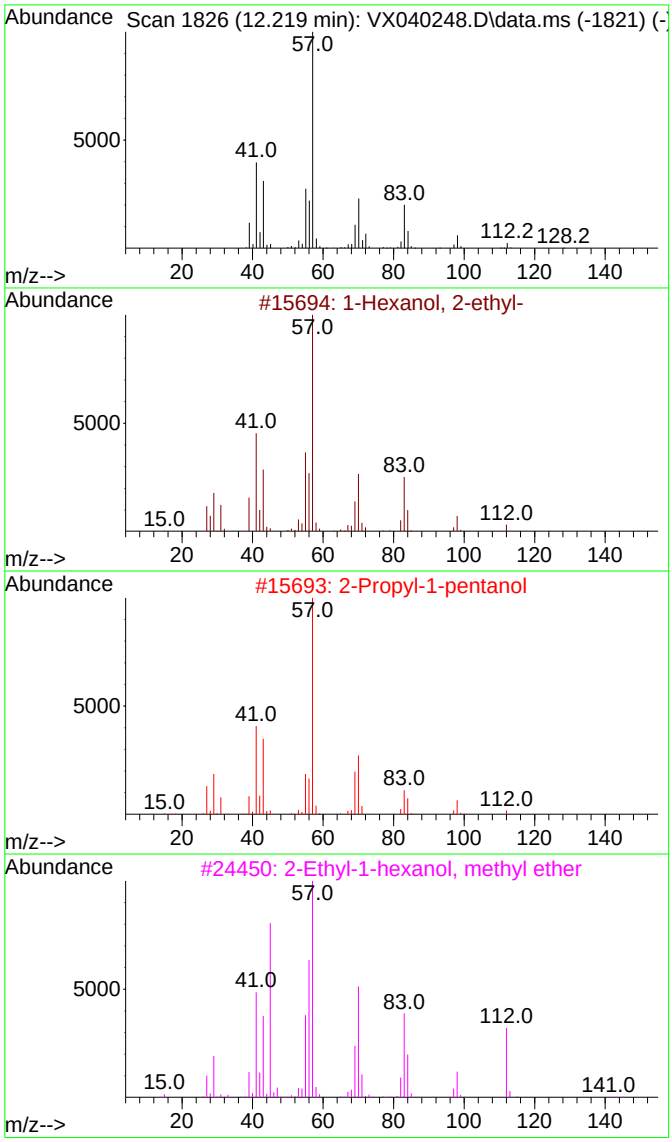
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

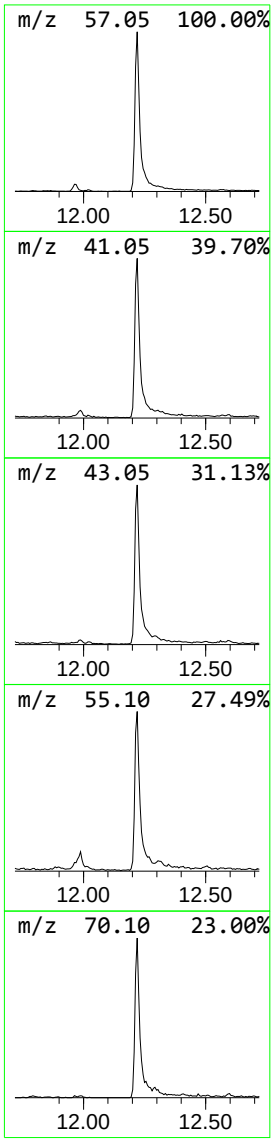
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	61.06 ug/l	526688	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	78
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
3	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
4	Oxalic acid, isobutyl octyl ester	258	C14H26O4	1000309-37-3	47
5	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	45





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021524\
Data File : VX040248.D
Acq On : 15 Feb 2024 13:42
Operator : JC/MD
Sample : P1424-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1285

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.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
Propane	1.148	9.0	ug/l	40146	1	5.550	223610	50.0
Ethanol	2.050	6.5	ug/l	28847	1	5.550	223610	50.0
Butanal	4.227	17.2	ug/l	77065	1	5.550	223610	50.0
1-Butanol	7.214	5.6	ug/l	33698	2	6.757	302183	50.0
4-Heptanol	10.750	16.6	ug/l	132027	3	10.055	398748	50.0
4-Heptanol, 3-m...	11.573	5.8	ug/l	50117	4	12.018	431293	50.0
3-Hexanol, 2,2-...	11.604	6.0	ug/l	51756	4	12.018	431293	50.0
Butanoic acid, ...	11.683	77.3	ug/l	666891	4	12.018	431293	50.0
1-Hexanol, 2-et...	12.219	61.1	ug/l	526688	4	12.018	431293	50.0