LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040236.D
Acq On : 14 Feb 2024 21:16
Operator : JC/MD
Sample : P1424-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 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: VX040236.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	44118	45505	6.23%	0.918%
2	1.368	40	46	50	rBV2	10856	14891	2.04%	0.300%
3	1.453	57	60	65	rVB	8464	9090	1.24%	0.183%
4	2.051	153	158	170	rBV	52607	87440	11.97%	1.764%
5	2.374	203	211	217	rBV	20469	33994	4.65%	0.686%
6	2.526	229	236	245	rBV	6942	14099	1.93%	0.284%
7	2.709	258	266	272	rBV2	4809	9710	1.33%	0.196%
8	2.953	299	306	319	rVB2	3869	8420	1.15%	0.170%
9	4.227	505	515	528	rBV	31655	87359	11.96%	1.762%
10	4.568	562	571	582	rBV2	4459	12418	1.70%	0.250%
11	5.385	693	705	717	rBV	46492	138651	18.98%	2.797%
12	5.550	723	732	745	rVB	80180	224686	30.75%	4.532%
13	5.952	788	798	808	rBV2	52441	139537	19.10%	2.815%
14	6.032	808	811	820	rVB4	3663	9506	1.30%	0.192%
15	6.763	921	931	946	rBV	125117	302213	41.36%	6.096%
16	7.208	997	1004	1021	rBV2	11490	35299	4.83%	0.712%
17	8.647	1233	1240	1247	rBV	268131	416338	56.98%	8.398%
18	8.720	1247	1252	1257	rVV	54398	86898	11.89%	1.753%
19	8.769	1257	1260	1270	rVB4	3849	9249	1.27%	0.187%
20	10.055	1463	1471	1483	rBV	277184	399028	54.61%	8.049%
21	10.159	1483	1488	1490	rVV2	8658	13160	1.80%	0.265%
22	10.195	1490	1494	1506	rVV	18099	32562	4.46%	0.657%
23	10.299	1506	1511	1519	rVB	61479	84048	11.50%	1.695%
24	10.506	1541	1545	1554	rVB	11831	16404	2.25%	0.331%
25	10.640	1561	1567	1571	rBV	22519	29856	4.09%	0.602%
26	10.683	1571	1574	1581	rVB	17346	21801	2.98%	0.440%
27	10.750	1581	1585	1594	rBV	85569	138576	18.97%	2.795%
28	11.079	1634	1639	1644	rBV	250457	319679	43.75%	6.449%
29	11.128	1644	1647	1654	rVB	20794	28375	3.88%	0.572%
30	11.232	1660	1664	1668	rBV2	6279	7717	1.06%	0.156%
31	11.281	1668	1672	1674	rBV2	8814	11400	1.56%	0.230%
32	11.305	1674	1676	1682	rVB3	8050	10935	1.50%	0.221%
33	11.384	1682	1689	1693	rBV2	20944	40115	5.49%	0.809%
34	11.451	1698	1700	1708	rVB	9977	12694	1.74%	0.256%
35	11.573	1715	1720	1722	rBV	38302	47268	6.47%	0.953%
36	11.604	1722	1725	1733	rVV3	39221	70057	9.59%	1.413%

LSC Area Percent Report

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ALS Vial : 25 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	11.683	1733	1738	1745	rVV	645664	730664	100.00%	14.739%
38	11.750	1745	1749	1755	rVB	35510	42973	5.88%	0.867%
39	11.969	1779	1785	1786	rBV	16325	21778	2.98%	0.439%
40	12.018	1789	1793	1800	rVV	340211	440285	60.26%	8.881%
41	12.085	1800	1804	1808	rVB	7732	10426	1.43%	0.210%
42	12.219	1821	1826	1837	rBV	370761	567798	77.71%	11.454%
43	12.597	1885	1888	1894	rVB4	6431	12052	1.65%	0.243%
44	13.292	1998	2002	2008	rVB4	6716	9921	1.36%	0.200%
45	13.597	2045	2052	2060	rBV9	7381	19508	2.67%	0.394%
46	13.676	2060	2065	2070	rVV	38489	46294	6.34%	0.934%
47	13.774	2076	2081	2088	rBV	10392	17347	2.37%	0.350%
48	14.030	2119	2123	2127	rVB2	7447	9033	1.24%	0.182%
49	14.140	2136	2141	2145	rBV3	6580	8842	1.21%	0.178%
50	14.225	2149	2155	2159	rVV4	3917	7437	1.02%	0.150%
51	14.274	2159	2163	2168	rVB2	8473	11155	1.53%	0.225%
52	14.634	2216	2222	2227	rBV	15684	23683	3.24%	0.478%
53	14.780	2241	2246	2251	rBV	6935	9175	1.26%	0.185%

Sum of corrected areas: 4957349

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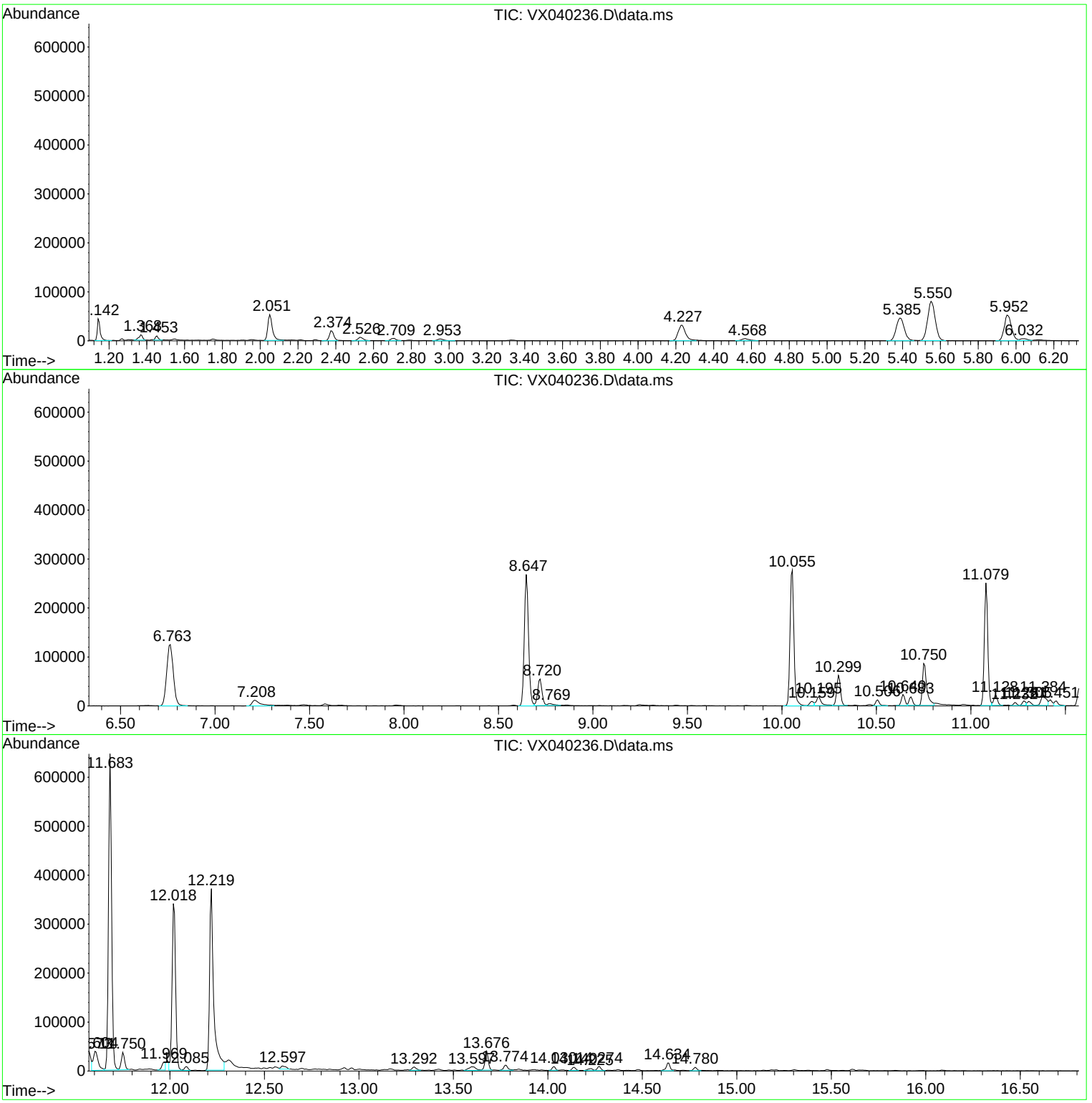
ALS Vial : 25 Sample Multiplier: 1

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040236.D
Acq On : 14 Feb 2024 21:16
Operator : JC/MD
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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

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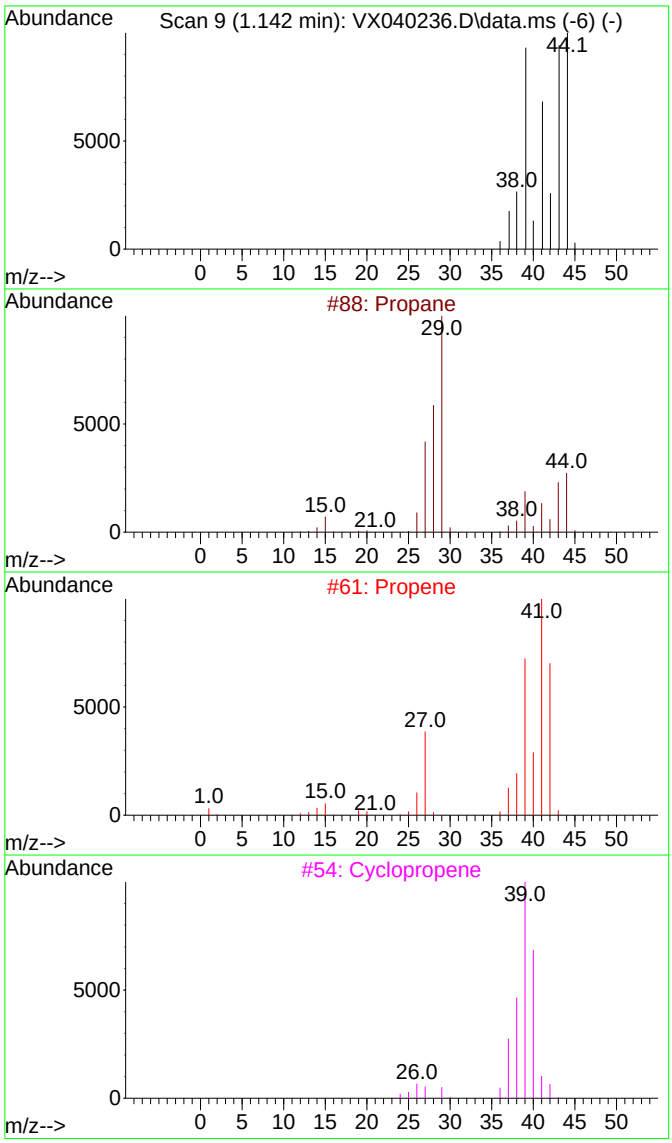
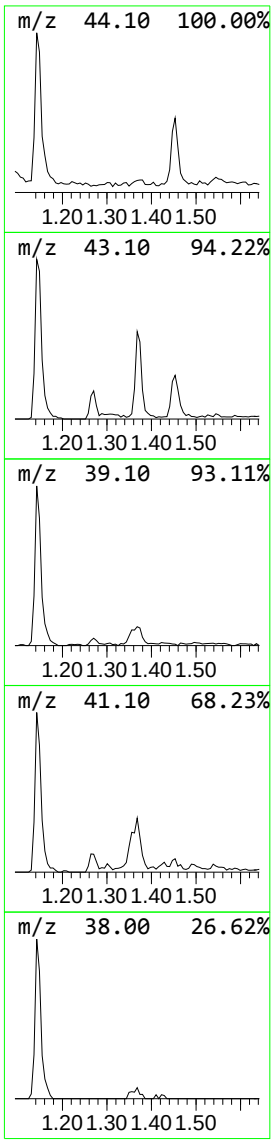
Peak Number 1 Propane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	10.13 ug/l	45505	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	83
2	Propene	42	C3H6	000115-07-1	9
3	Cyclopropene	40	C3H4	002781-85-3	4
4	Alanine	89	C3H7NO2	000056-41-7	2
5	Ethanamine, 2-propoxy-	103	C5H13NO	042185-03-5	2





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040236.D
Acq On : 14 Feb 2024 21:16
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 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

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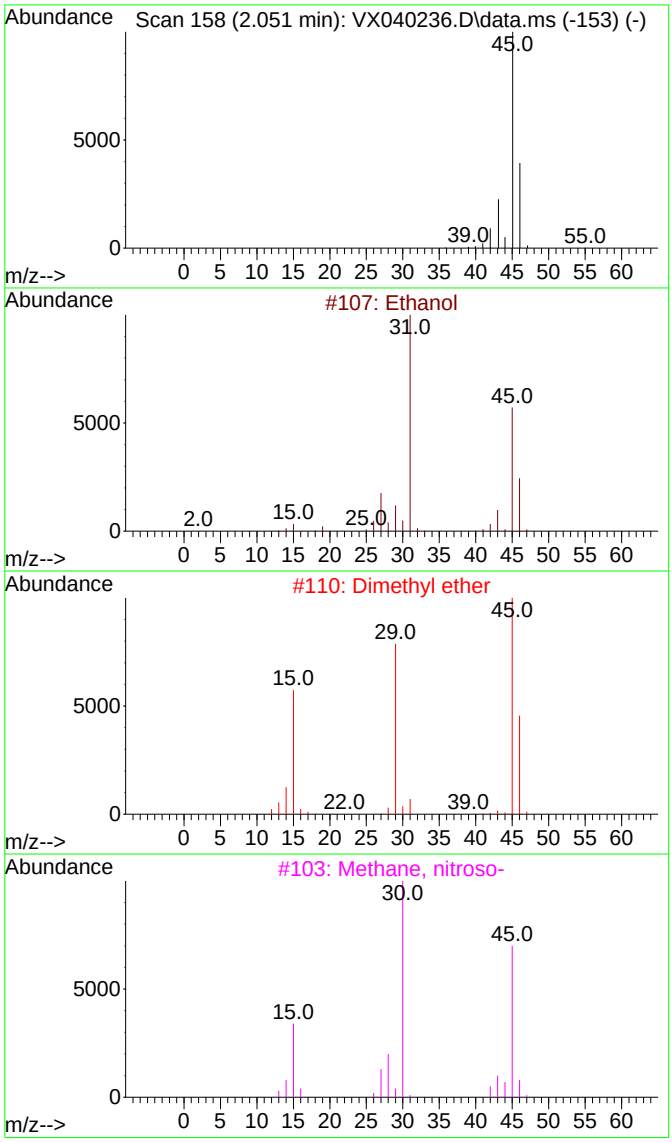
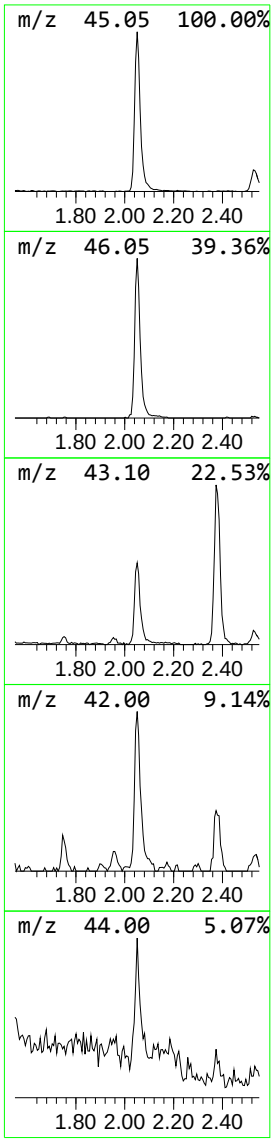
Peak Number 2 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.051	19.46 ug/l	87440	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	Oxalic acid	90	C2H2O4	000144-62-7	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040236.D
Acq On : 14 Feb 2024 21:16
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 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

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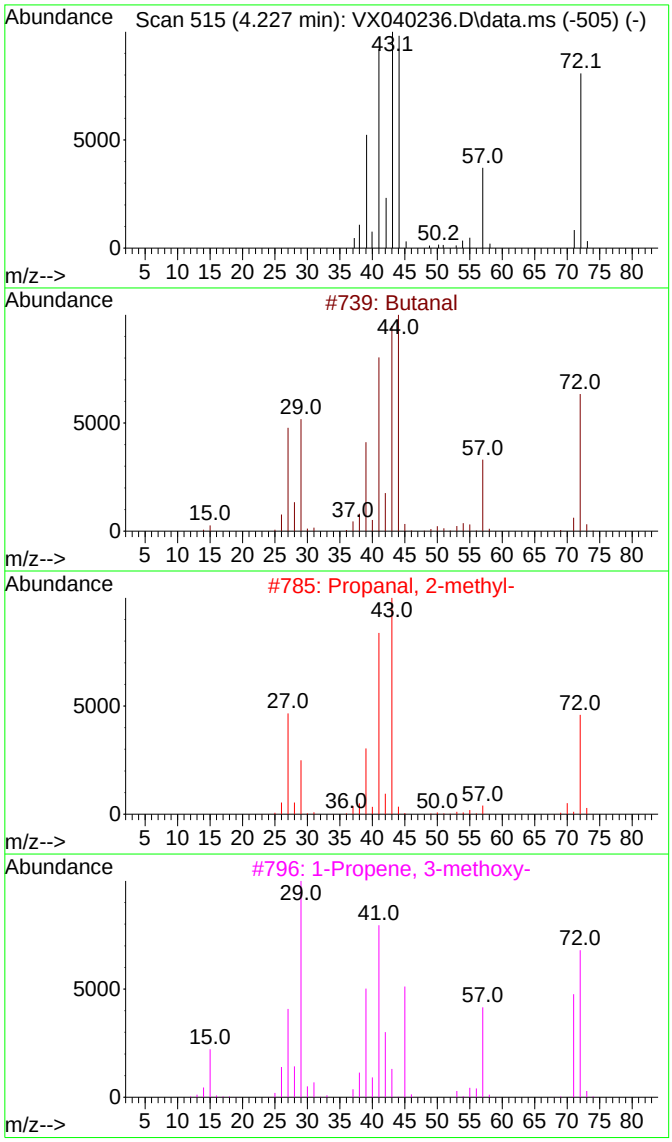
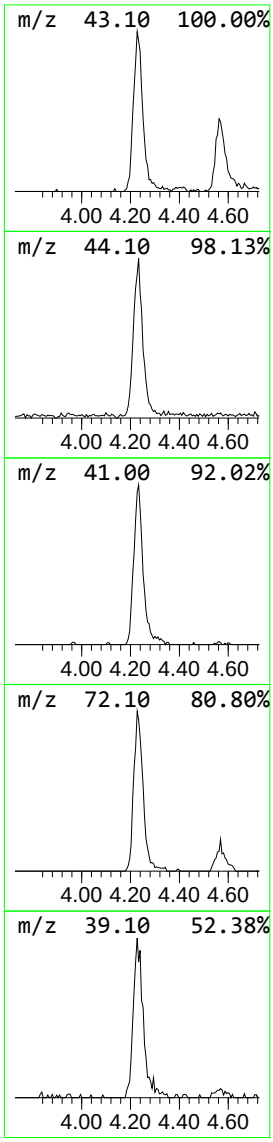
Peak Number 3 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	19.44 ug/l	87359	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
3	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37
4	Ethene, ethoxy-	72	C4H8O	000109-92-2	33
5	2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040236.D
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Operator : JC/MD
Sample : P1424-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1285

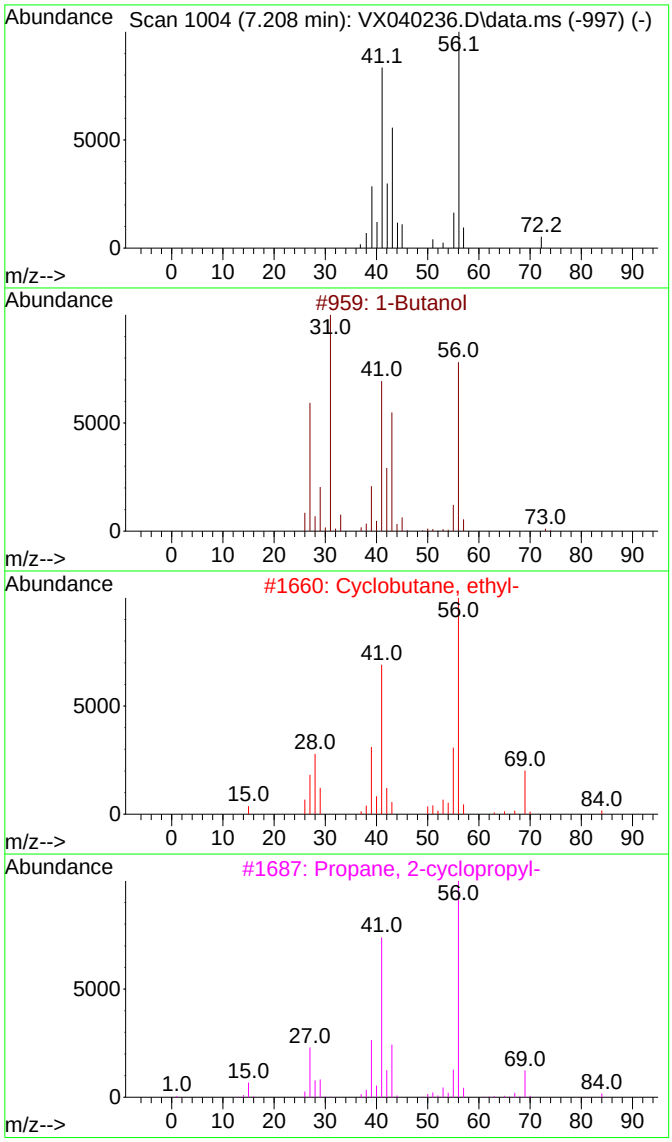
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

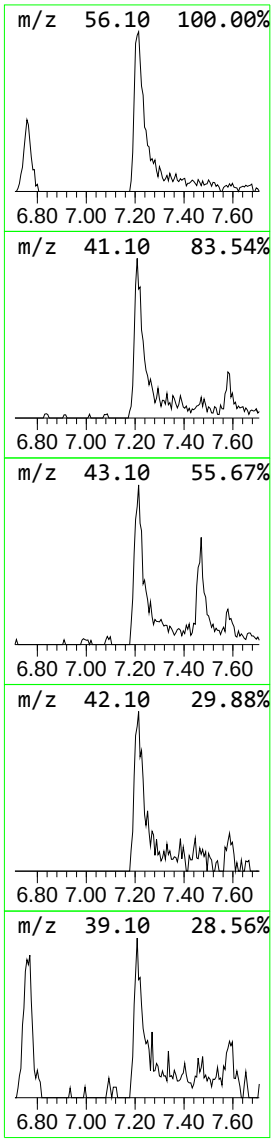
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Butanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	5.84 ug/l	35299	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	72
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	38
3	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	36
4	Pentane	72	C5H12	000109-66-0	9
5	1-Amino-3-methylbutan-2-ol	103	C5H13NO	1000486-88-4	9





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ALS Vial : 25 Sample Multiplier: 1

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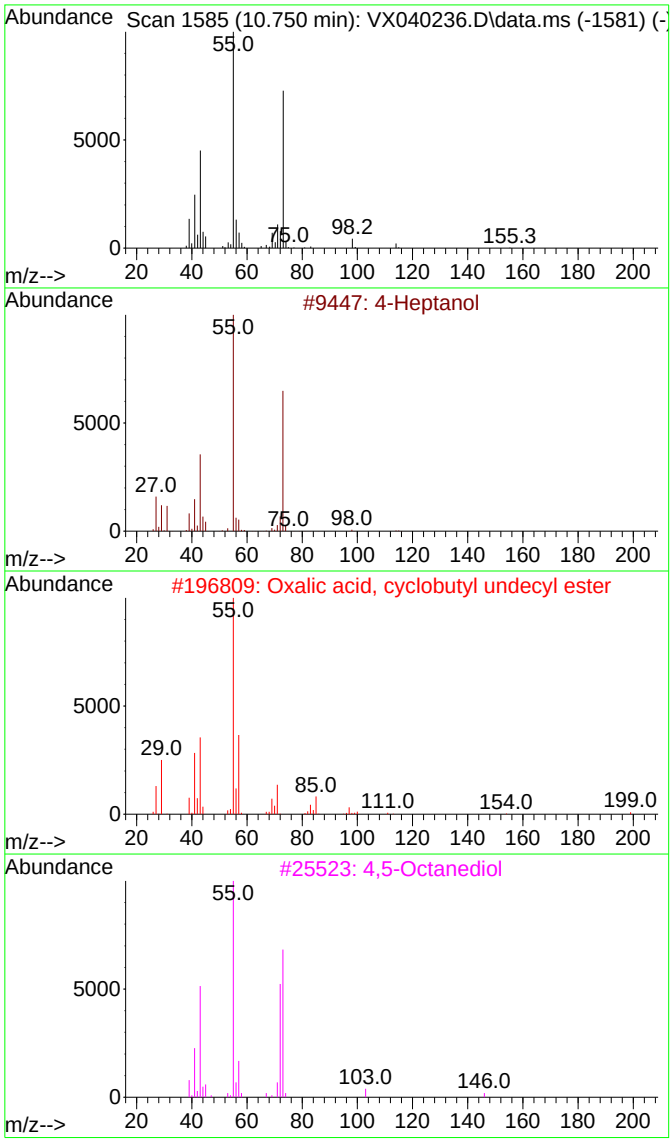
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

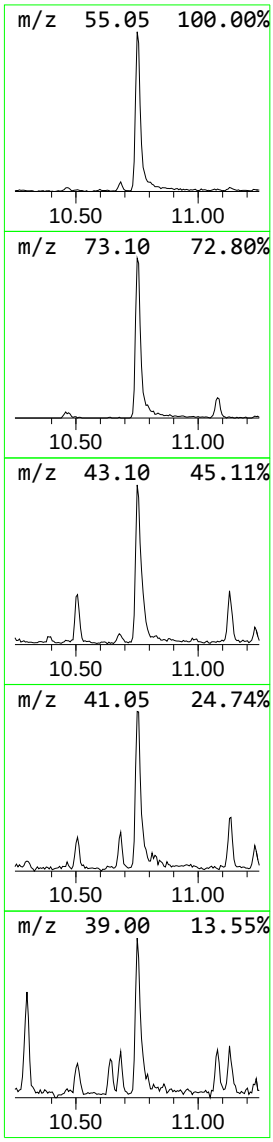
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.750	17.36 ug/l	138576	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol	116	C7H16O	000589-55-9	59
2	Oxalic acid, cyclobutyl undecyl ...	298	C17H30O4	1000309-70-2	43
3	4,5-Octanediol	146	C8H18O2	022607-10-9	40
4	1-Hepten-4-ol	114	C7H14O	003521-91-3	40
5	Oxalic acid, cyclobutyl octyl ester	256	C14H24O4	1000309-69-9	37





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Operator : JC/MD
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ALS Vial : 25 Sample Multiplier: 1

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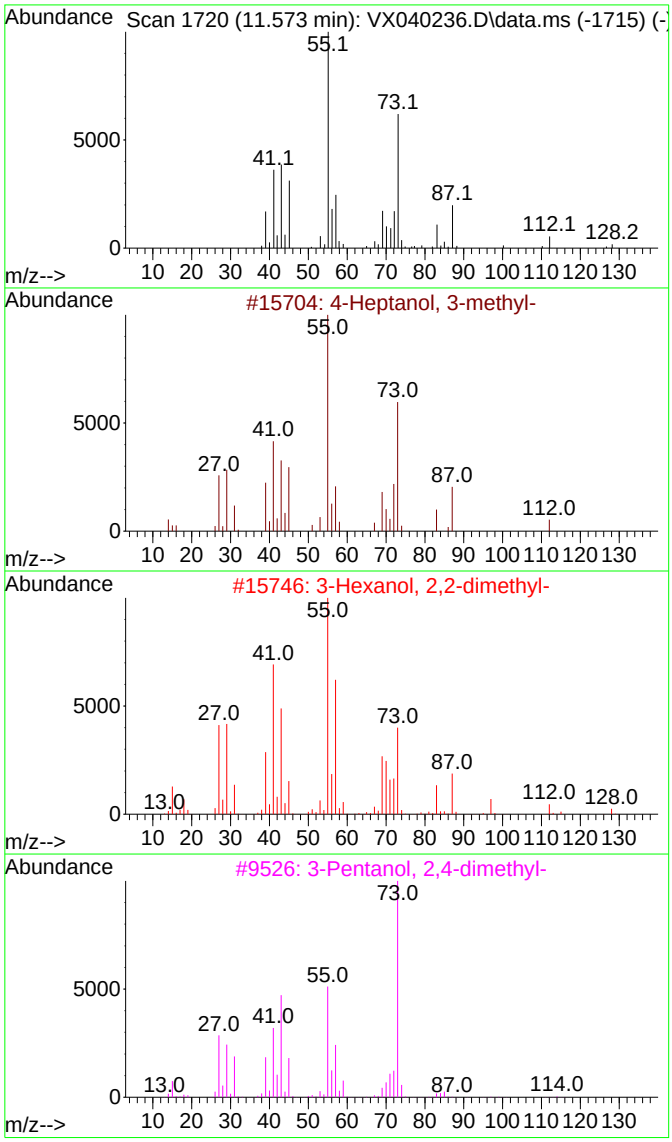
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

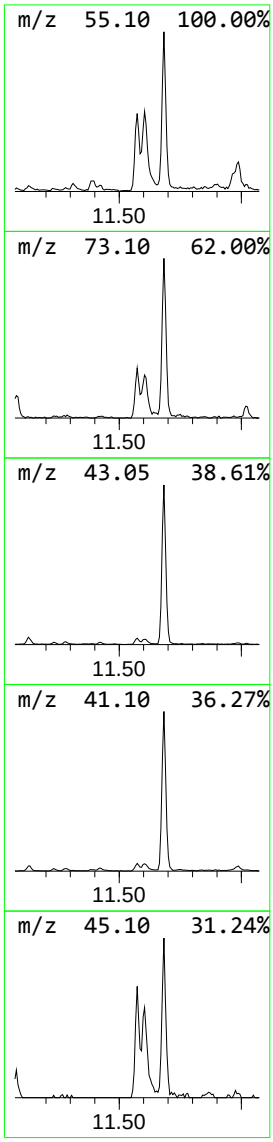
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 4-Heptanol, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.573	5.37 ug/l	47268	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 3-methyl-	130	C8H18O	001838-73-9	90
2	3-Hexanol, 2,2-dimethyl-	130	C8H18O	004209-90-9	47
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	38
4	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	32
5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	16





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ALS Vial : 25 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

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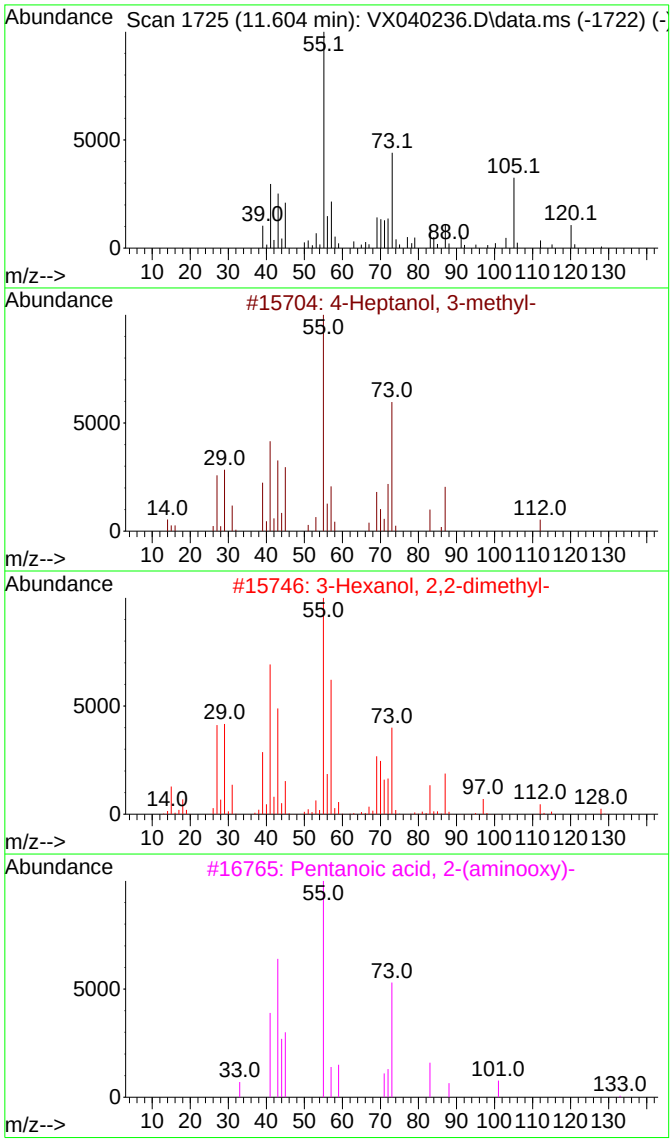
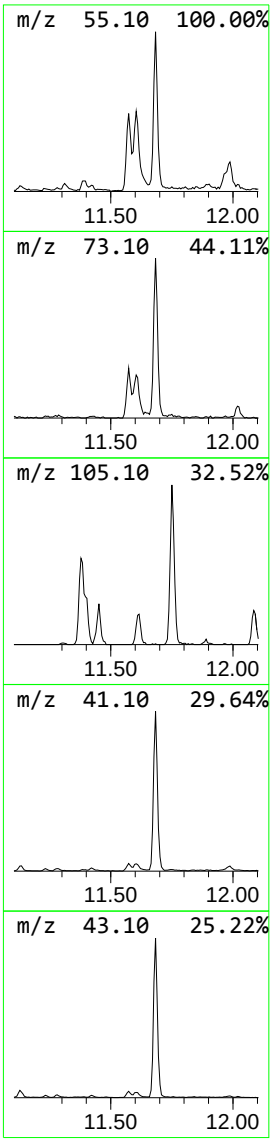
Peak Number 7 unknown11.604 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.604	7.96 ug/l	70057	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 3-methyl-	130	C8H18O	001838-73-9	47
2	3-Hexanol, 2,2-dimethyl-	130	C8H18O	004209-90-9	32
3	Pentanoic acid, 2-(aminooxy)-	133	C5H11NO3	005699-55-8	32
4	5-Methyl-4-octanol	144	C9H20O	059734-23-5	17
5	3,3-Dimethyl-4-heptanol	144	C9H20O	019549-78-1	17





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Data File : VX040236.D
Acq On : 14 Feb 2024 21:16
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1285

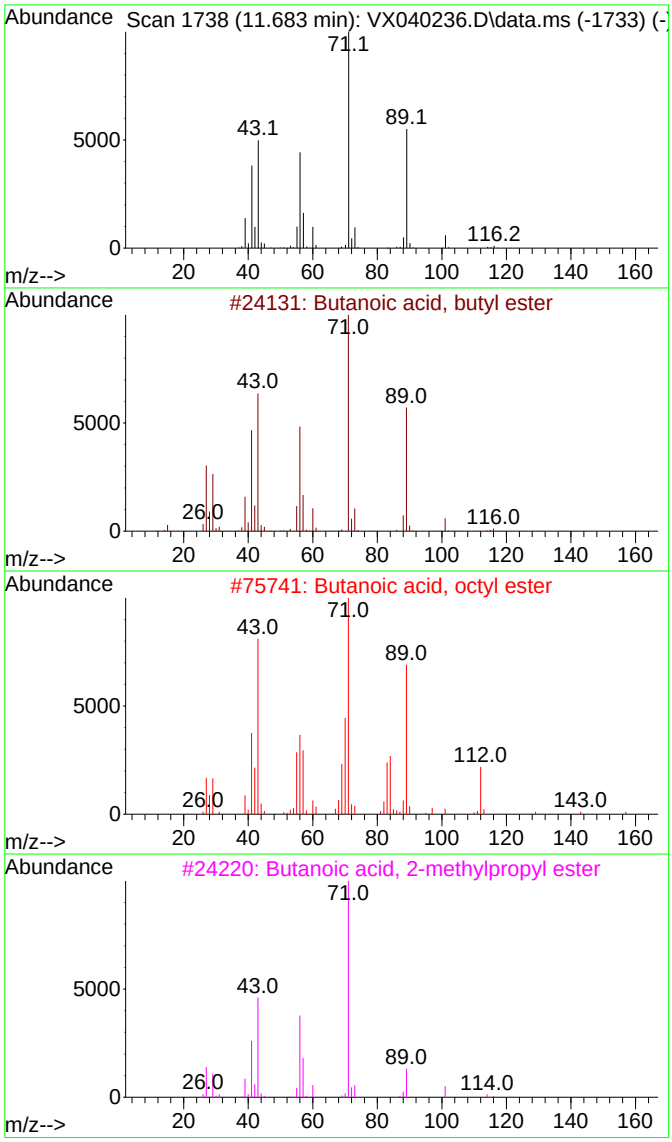
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

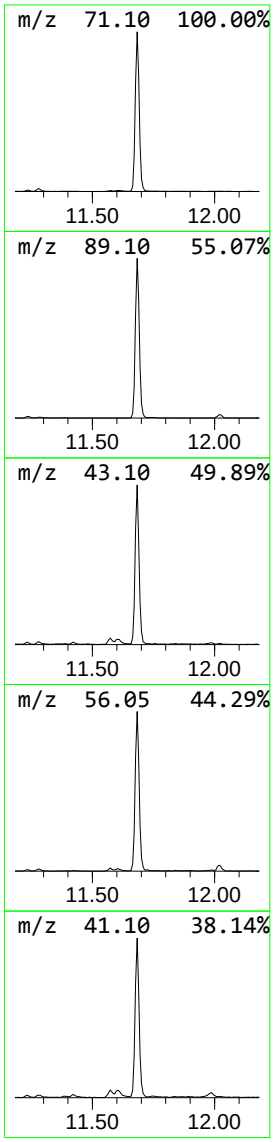
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	82.98 ug/l	730664	1,4-Dichlorobenzene-d4	12.024

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	64
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040236.D
Acq On : 14 Feb 2024 21:16
Operator : JC/MD
Sample : P1424-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1285

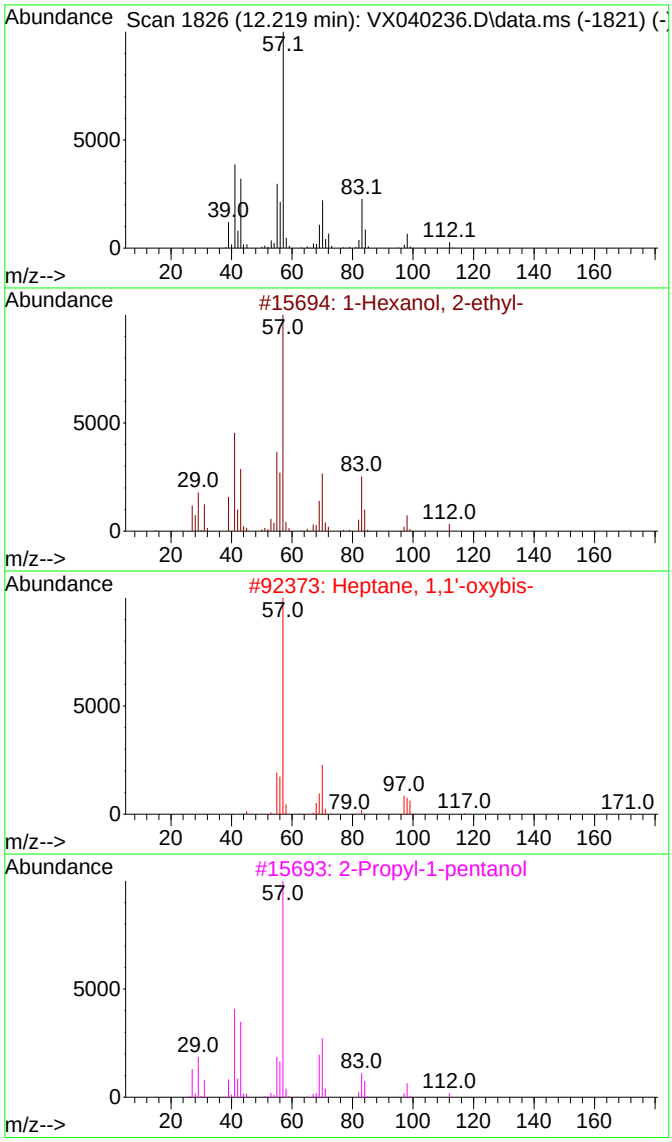
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X020924W.M
Quant Title : SW846 8260

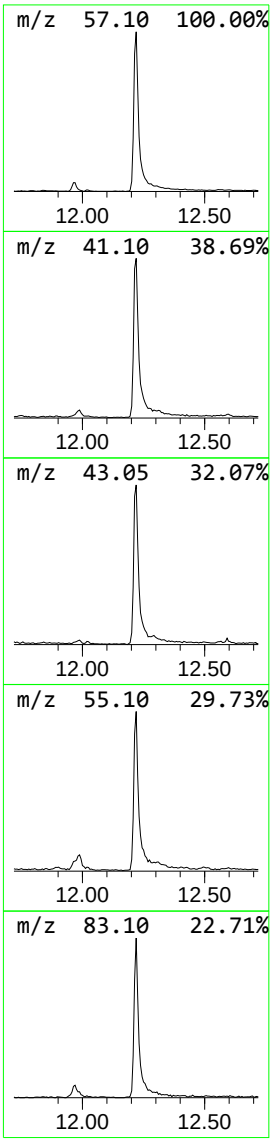
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	64.48 ug/l	567798	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	90
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
4	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
5	Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040236.D
Acq On : 14 Feb 2024 21:16
Operator : JC/MD
Sample : P1424-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1285

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

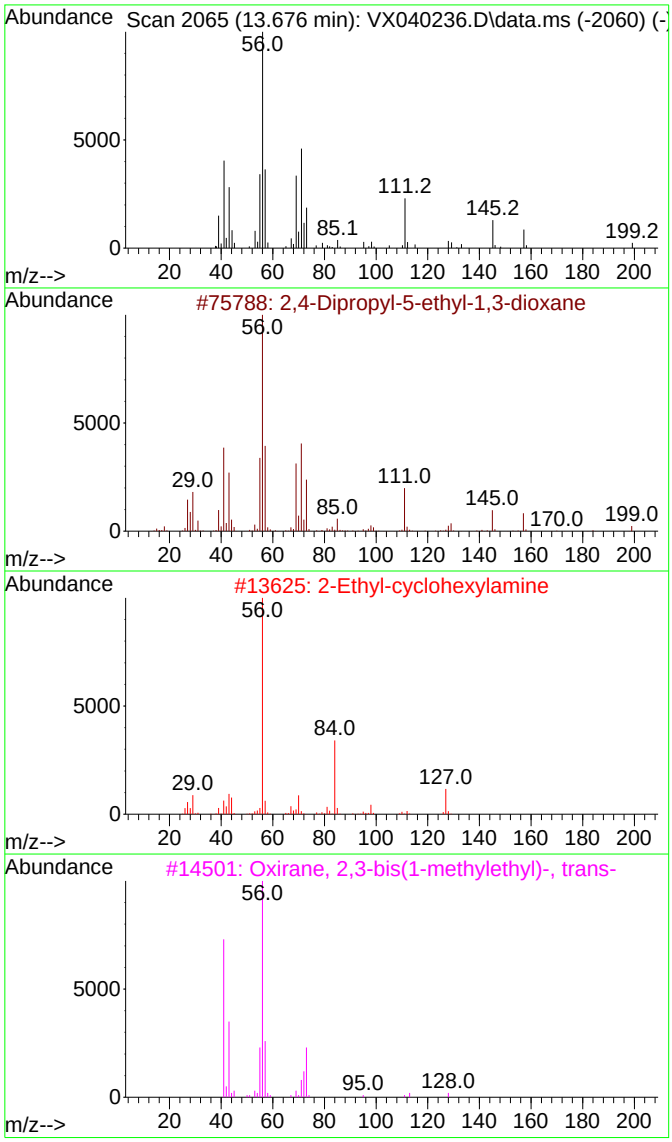
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

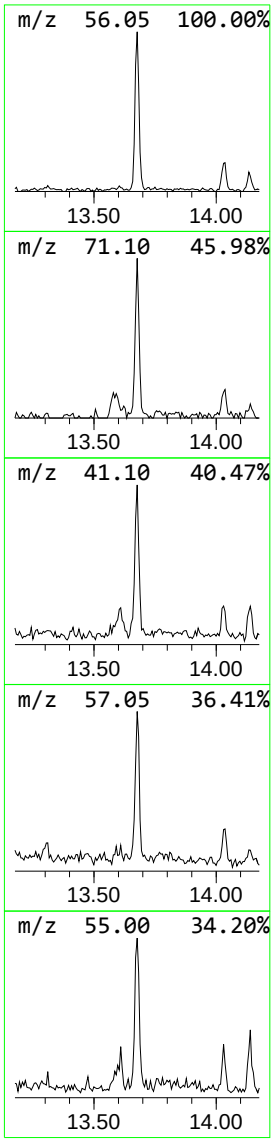
****

Peak Number 10 unknown13.677 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.677	5.26 ug/l	46294	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	43
2	2-Ethyl-cyclohexylamine	127	C8H17N	024216-90-8	35
3	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	32
4	Cyclopentanone, 2,2,5,5-tetramet...	140	C9H16O	004541-35-9	32
5	1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021424\
Data File : VX040236.D
Acq On : 14 Feb 2024 21:16
Operator : JC/MD
Sample : P1424-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 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	1.142	10.1	ug/l	45505	1	5.550	224686	50.0
Ethanol	2.051	19.5	ug/l	87440	1	5.550	224686	50.0
Butanal	4.227	19.4	ug/l	87359	1	5.550	224686	50.0
1-Butanol	7.208	5.8	ug/l	35299	2	6.763	302213	50.0
4-Heptanol	10.750	17.4	ug/l	138576	3	10.055	399028	50.0
4-Heptanol, 3-m...	11.573	5.4	ug/l	47268	4	12.024	440285	50.0
unknown11.604	11.604	8.0	ug/l	70057	4	12.024	440285	50.0
Butanoic acid, ...	11.683	83.0	ug/l	730664	4	12.024	440285	50.0
1-Hexanol, 2-et...	12.219	64.5	ug/l	567798	4	12.024	440285	50.0
unknown13.677	13.677	5.3	ug/l	46294	4	12.024	440285	50.0