LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013124\
Data File : VX040052.D
Acq On : 31 Jan 2024 17:00
Operator : JC/MD
Sample : P1282-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1241

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\82X013024W.M
Title : SW846 8260

Signal : TIC: VX040052.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	19	rVB	57360	59741	3.60%	0.728%
2	1.447	56	59	71	rBV	1424059	1658443	100.00%	20.203%
3	2.050	150	158	170	rBV	30029	50306	3.03%	0.613%
4	2.288	191	197	206	rBV	96234	154784	9.33%	1.886%
5	2.373	206	211	229	rVB	51316	86588	5.22%	1.055%
6	2.532	230	237	244	rBV	8657	17128	1.03%	0.209%
7	3.324	357	367	380	rBV2	9528	22394	1.35%	0.273%
8	4.227	505	515	531	rBV	70872	188971	11.39%	2.302%
9	4.562	560	570	585	rBV	10854	32741	1.97%	0.399%
10	5.385	695	705	719	rBV	54490	157183	9.48%	1.915%
11	5.550	722	732	753	rVB	87980	248506	14.98%	3.027%
12	5.958	789	799	809	rBV2	63667	169395	10.21%	2.064%
13	6.757	919	930	947	rBV	141826	351868	21.22%	4.286%
14	7.208	996	1004	1019	rBV	35872	91755	5.53%	1.118%
15	7.580	1059	1065	1073	rBV2	24361	48787	2.94%	0.594%
16	8.647	1234	1240	1248	rBV	315157	491191	29.62%	5.984%
17	8.769	1256	1260	1270	rVB	8717	16637	1.00%	0.203%
18	9.238	1332	1337	1347	rBV2	11436	23527	1.42%	0.287%
19	9.518	1379	1383	1392	rBV	33468	48827	2.94%	0.595%
20	10.055	1464	1471	1482	rBV	334281	467201	28.17%	5.691%
21	10.152	1482	1487	1492	rBV2	16103	25650	1.55%	0.312%
22	10.305	1508	1512	1519	rVB2	21623	34113	2.06%	0.416%
23	10.445	1528	1535	1541	rBV3	20522	30827	1.86%	0.376%
24	10.506	1541	1545	1551	rVB	15367	20644	1.24%	0.251%
25	10.683	1570	1574	1581	rVB	44095	60276	3.63%	0.734%
26	10.750	1581	1585	1595	rBV2	114871	184272	11.11%	2.245%
27	11.079	1634	1639	1644	rBV	292422	362356	21.85%	4.414%
28	11.134	1644	1648	1655	rVB2	18485	27835	1.68%	0.339%
29	11.280	1668	1672	1675	rBV	16191	21195	1.28%	0.258%
30	11.573	1714	1720	1722	rBV2	47147	59732	3.60%	0.728%
31	11.603	1722	1725	1733	rVV	49433	82068	4.95%	1.000%
32	11.683	1733	1738	1746	rVV	894976	1022751	61.67%	12.459%
33	11.987	1781	1788	1790	rBV	123997	154608	9.32%	1.883%
34	12.018	1790	1793	1802	rVB	391429	520556	31.39%	6.341%
35	12.219	1820	1826	1836	rBV	693182	937112	56.51%	11.416%
36	12.305	1836	1840	1849	rVV6	34867	81517	4.92%	0.993%

LSC Area Percent Report

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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1241

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\82X013024W.M
Title : SW846 8260

37	12.414	1853	1858	1863	rVB	33300	45503	2.74%	0.554%
38	12.597	1884	1888	1893	rVB5	12523	19607	1.18%	0.239%
39	13.609	2046	2054	2060	rBV4	16760	30080	1.81%	0.366%
40	13.676	2060	2065	2070	rVV	50826	60470	3.65%	0.737%
41	14.030	2117	2123	2127	rBV2	15513	20310	1.22%	0.247%
42	14.140	2137	2141	2150	rVB	16471	21462	1.29%	0.261%

Sum of corrected areas: 8208917

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ClientSampleId :
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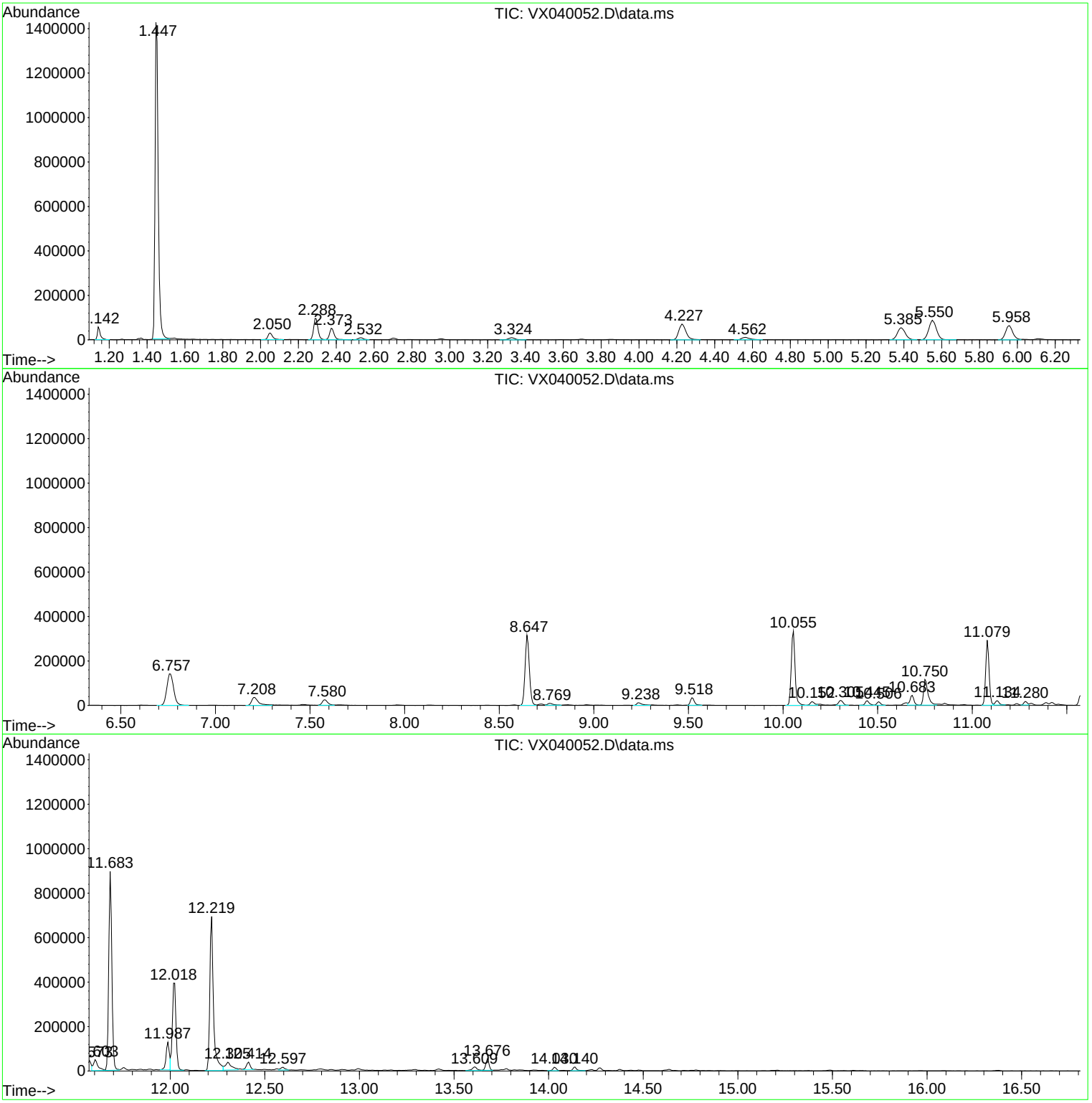
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

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



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Data File : VX040052.D
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

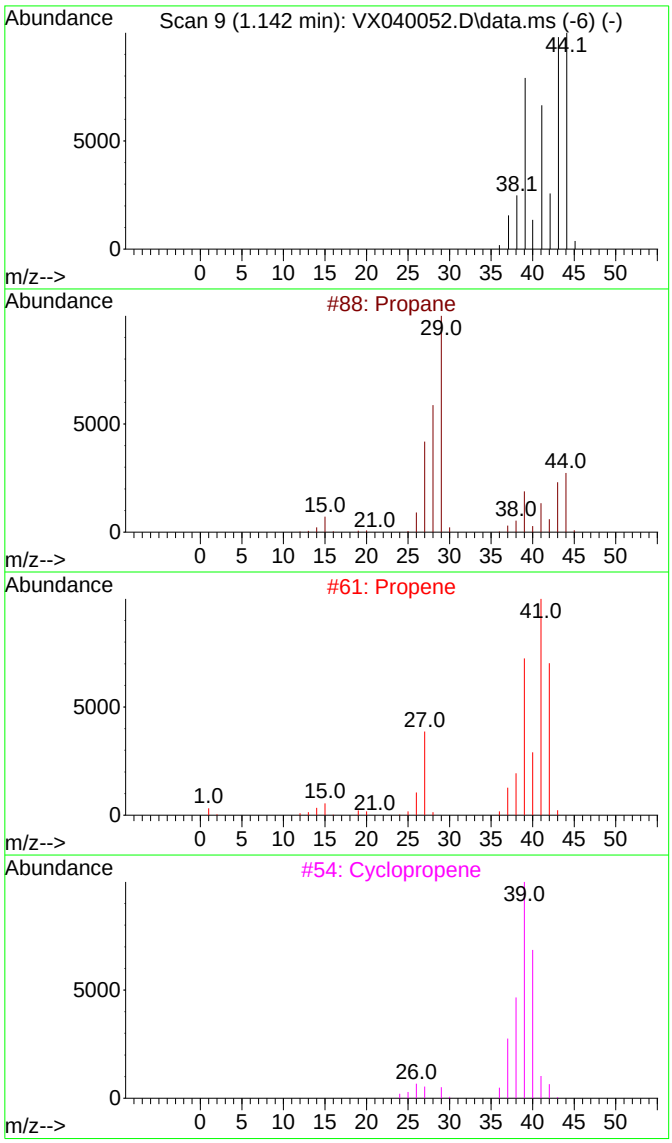
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

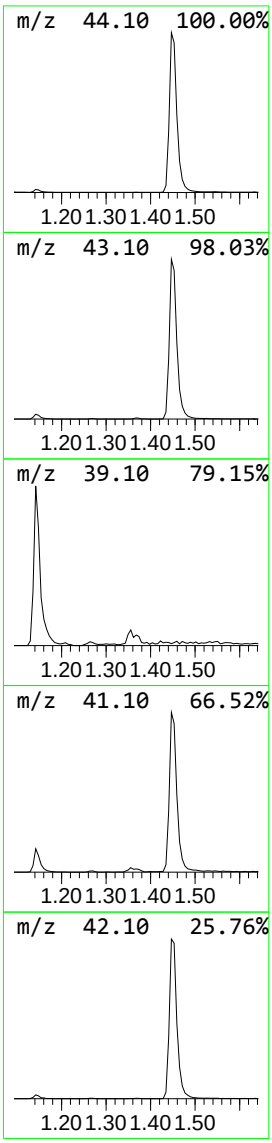
****

Peak Number 1 Propane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	12.02 ug/l	59741	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	90
2	Propene	42	C3H6	000115-07-1	9
3	Cyclopropene	40	C3H4	002781-85-3	2
4	Alanine	89	C3H7NO2	000056-41-7	2
5	Ethanamine, 2-propoxy-	103	C5H13NO	042185-03-5	2





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Data File : VX040052.D
Acq On : 31 Jan 2024 17:00
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1241

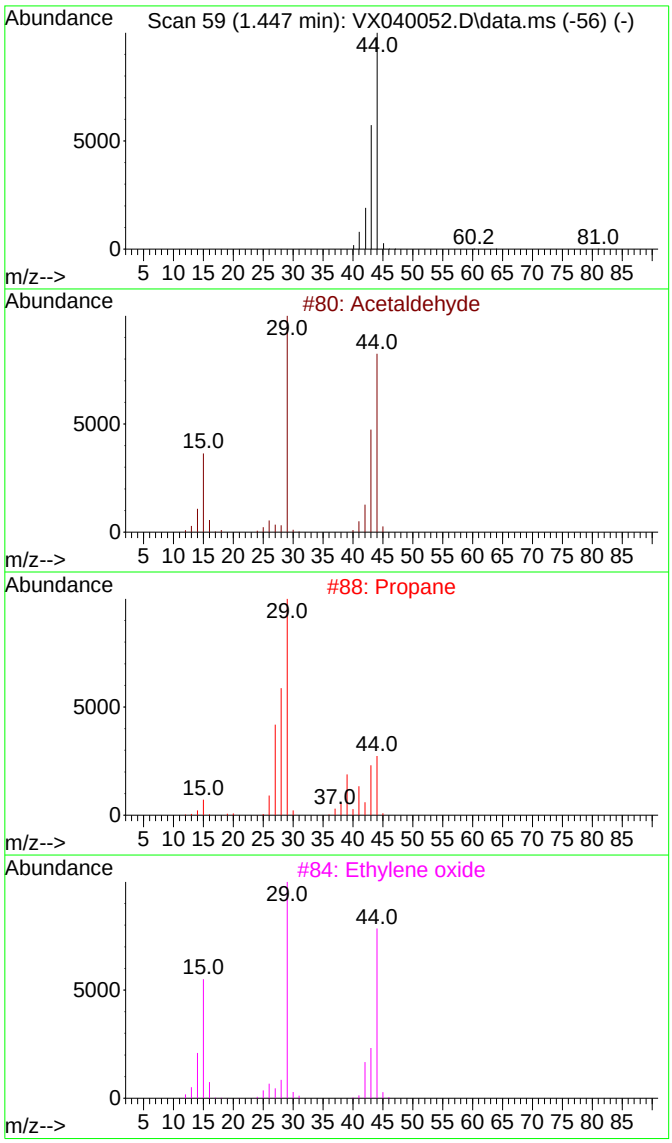
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

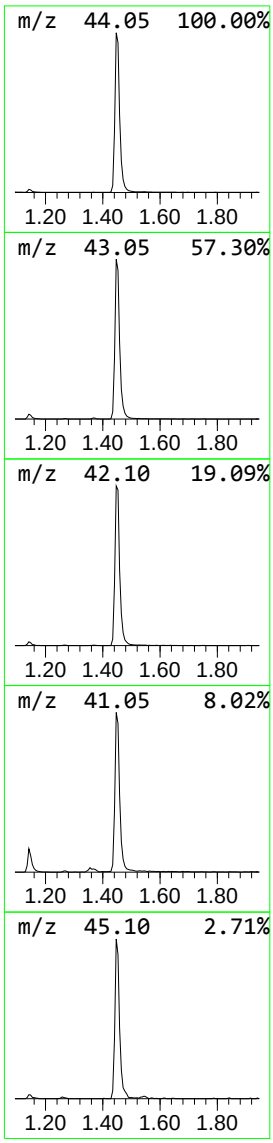
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.447	333.68 ug/l	1658440	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	74
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Alanine	89	C3H7NO2	000056-41-7	4
5	Hydrogen isocyanate	43	CHNO	000075-13-8	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013124\
Data File : VX040052.D
Acq On : 31 Jan 2024 17:00
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1241

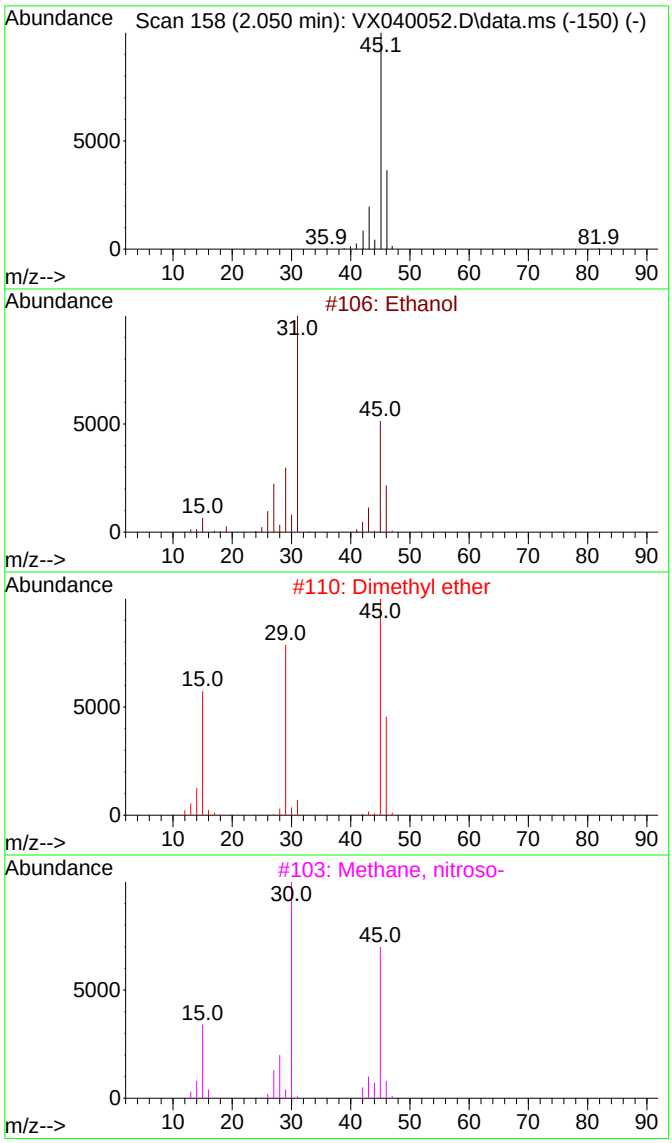
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

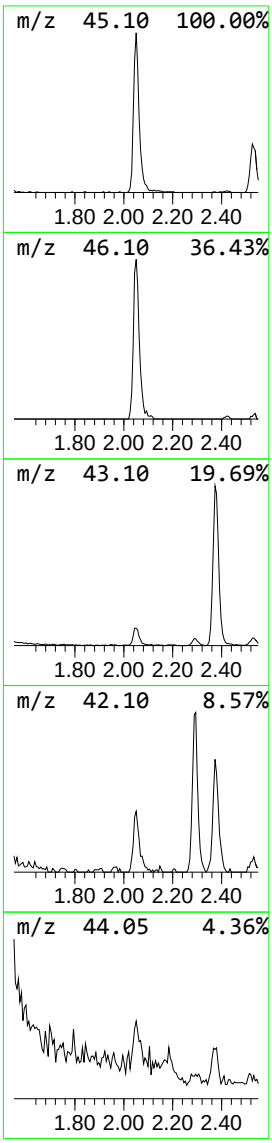
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.050	10.12 ug/l	50306	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	86
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	7
4	Propanedioic acid, dihydroxy-	136	C3H4O6	000560-27-0	4
5	Formic acid	46	CH2O2	000064-18-6	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013124\
Data File : VX040052.D
Acq On : 31 Jan 2024 17:00
Operator : JC/MD
Sample : P1282-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1241

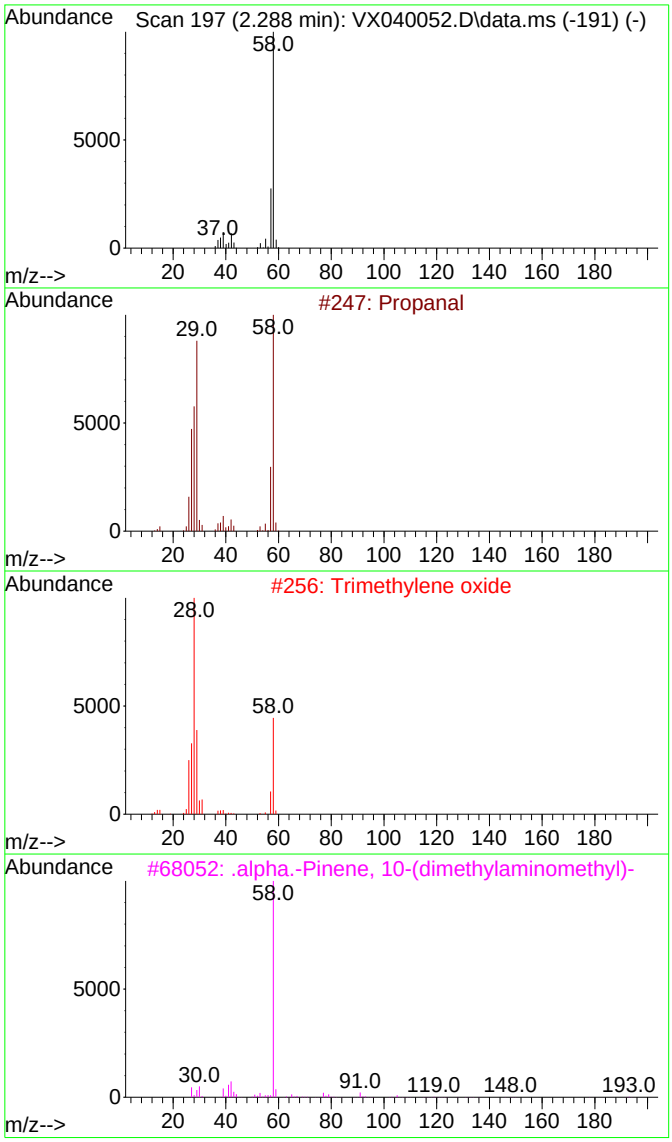
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

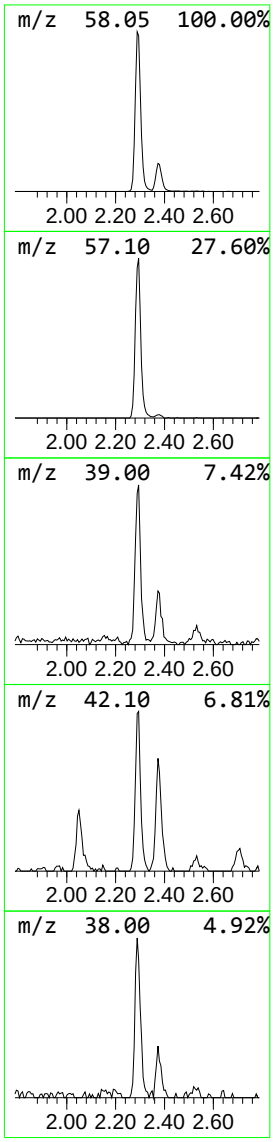
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Propanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.288	31.14 ug/l	154784	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	78
2	Trimethylene oxide	58	C3H6O	000503-30-0	9
3	.alpha.-Pinene, 10-(dimethylamin...	193	C13H23N	015063-97-5	9
4	Propylene oxide	58	C3H6O	000075-56-9	7
5	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013124\
Data File : VX040052.D
Acq On : 31 Jan 2024 17:00
Operator : JC/MD
Sample : P1282-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1241

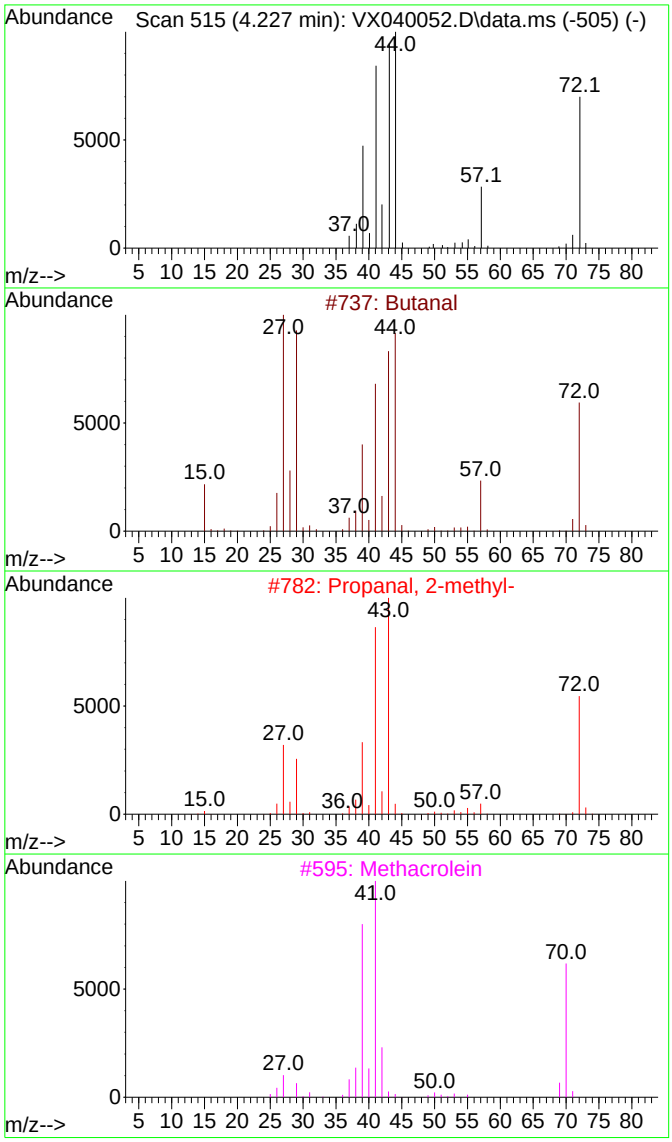
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

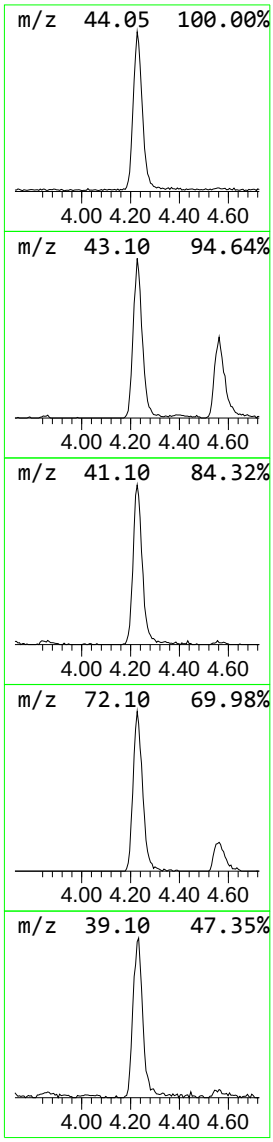
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	38.02 ug/l	188971	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	38
3	Methacrolein	70	C4H6O	000078-85-3	27
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	25
5	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	23





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Operator : JC/MD
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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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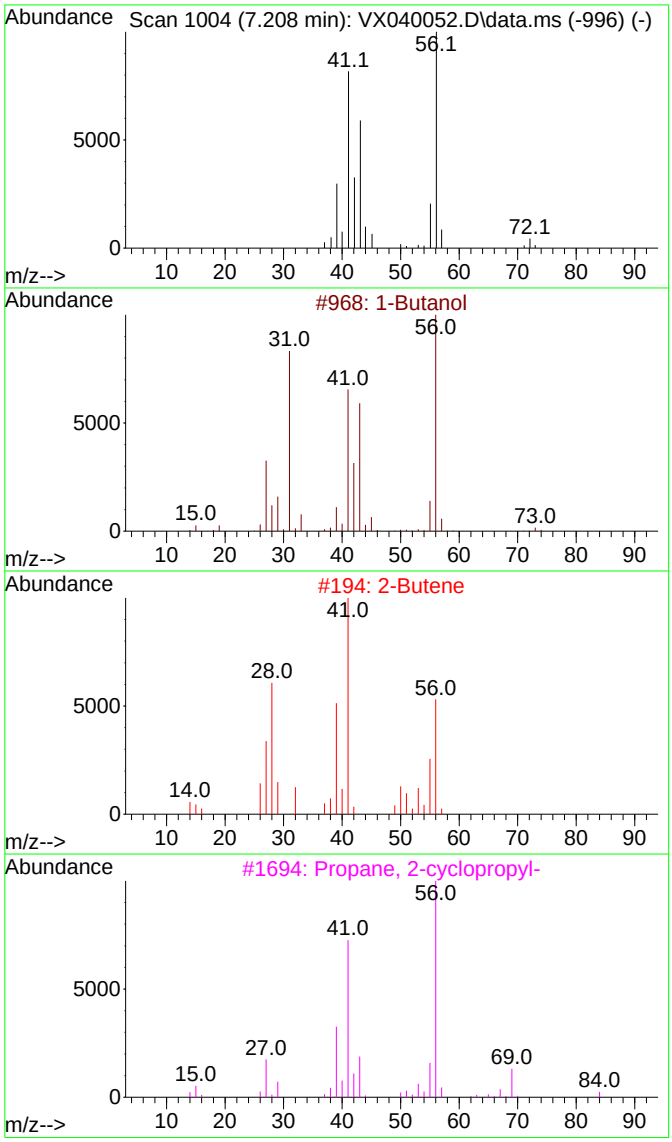
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

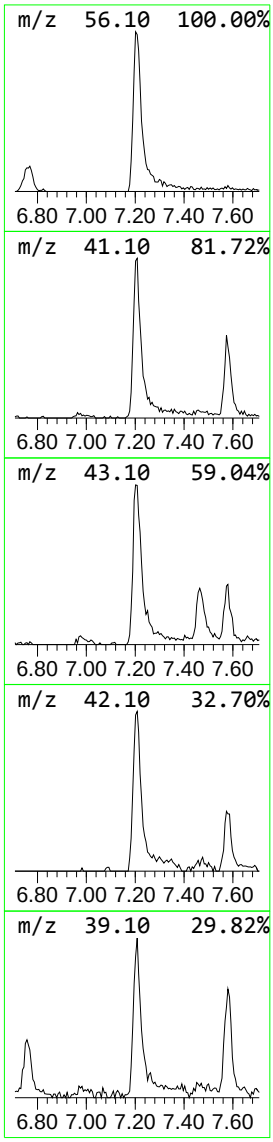
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Butanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	13.04 ug/l	91755	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	64
2	2-Butene	56	C4H8	000107-01-7	50
3	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	36
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	10
5	Pentane	72	C5H12	000109-66-0	10





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Operator : JC/MD
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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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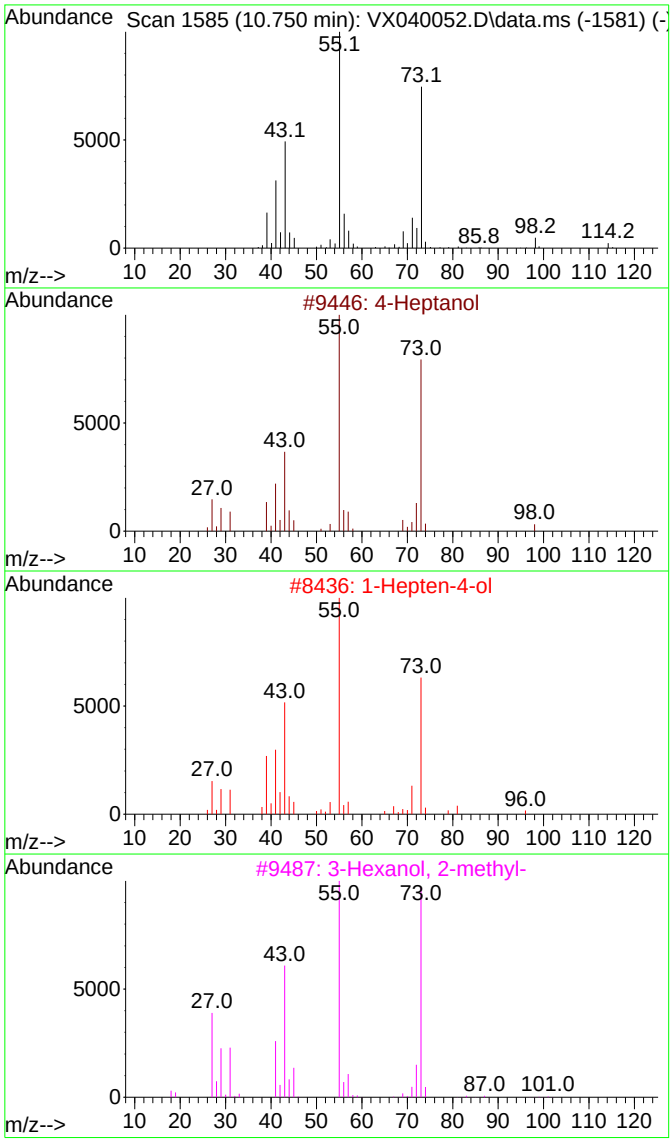
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

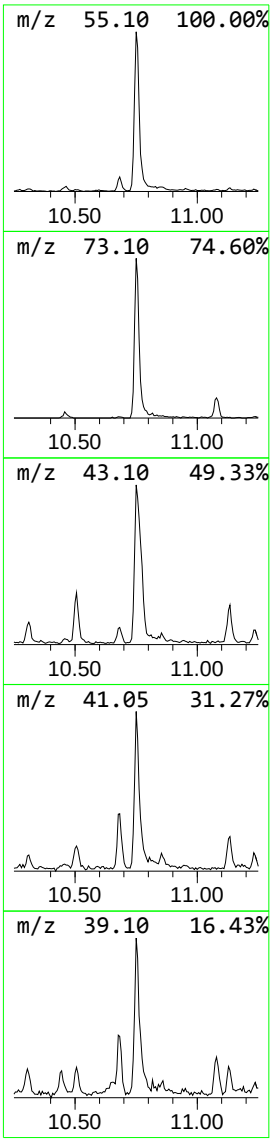
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4-Heptanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.750	19.72 ug/l	184272	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol	116	C7H16O	000589-55-9	59
2	1-Hepten-4-ol	114	C7H14O	003521-91-3	50
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	40
4	Oxalic acid, cyclobutyl heptyl e...	242	C13H22O4	1000309-69-8	38
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	37





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MSVOA_X
ClientSampleId :
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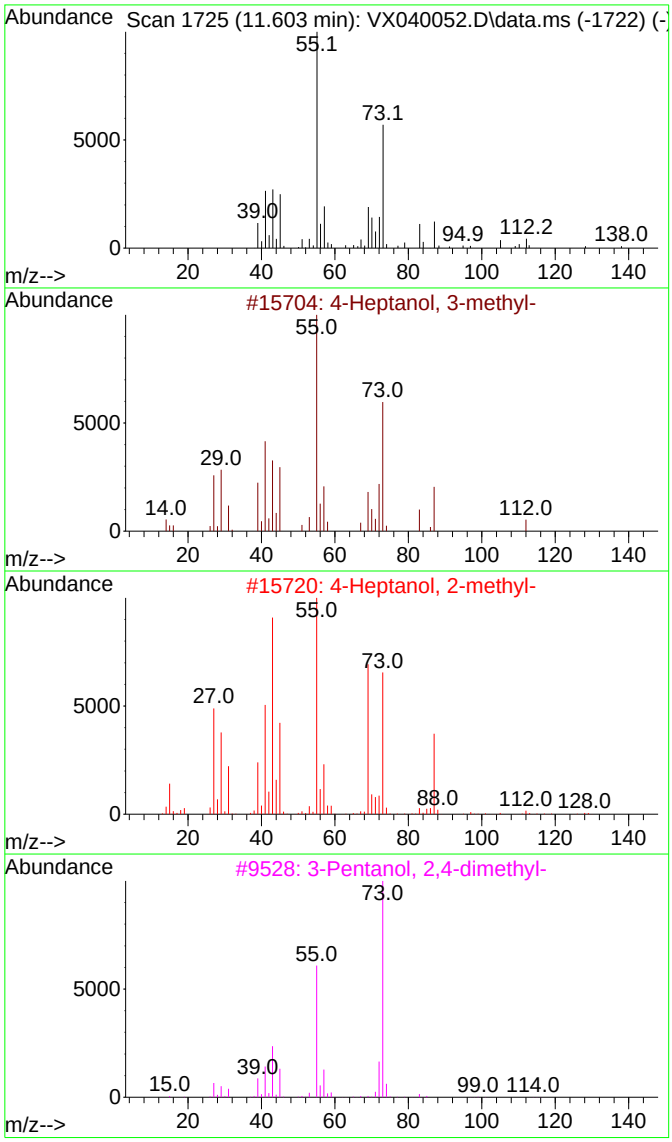
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

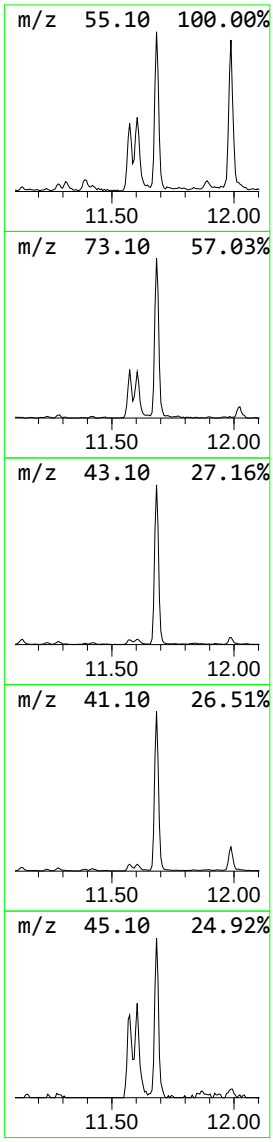
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 4-Heptanol, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.603	7.88 ug/l	82068	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	83
2	4-Heptanol, 2-methyl-	130	C8H18O	021570-35-4	53
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	47
4	Pentanoic acid, 2-(aminooxy)-	133	C5H11NO3	005699-55-8	42
5	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	35





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Data File : VX040052.D
Acq On : 31 Jan 2024 17:00
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Instrument :
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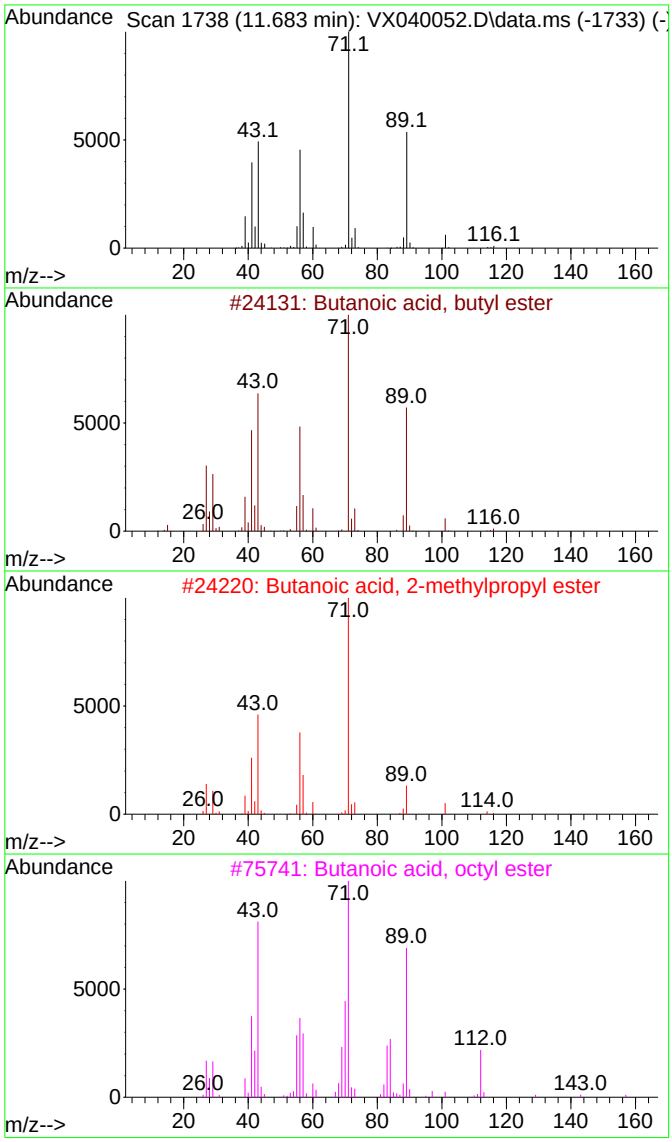
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

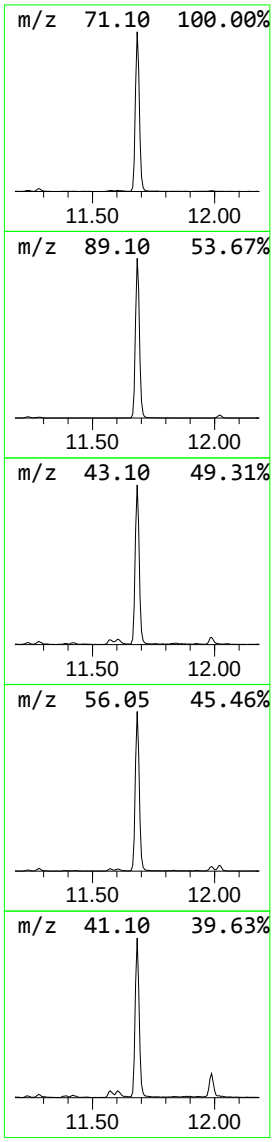
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Butanoic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	98.24 ug/l	1022750	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, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
3	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
4	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013124\
Data File : VX040052.D
Acq On : 31 Jan 2024 17:00
Operator : JC/MD
Sample : P1282-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1241

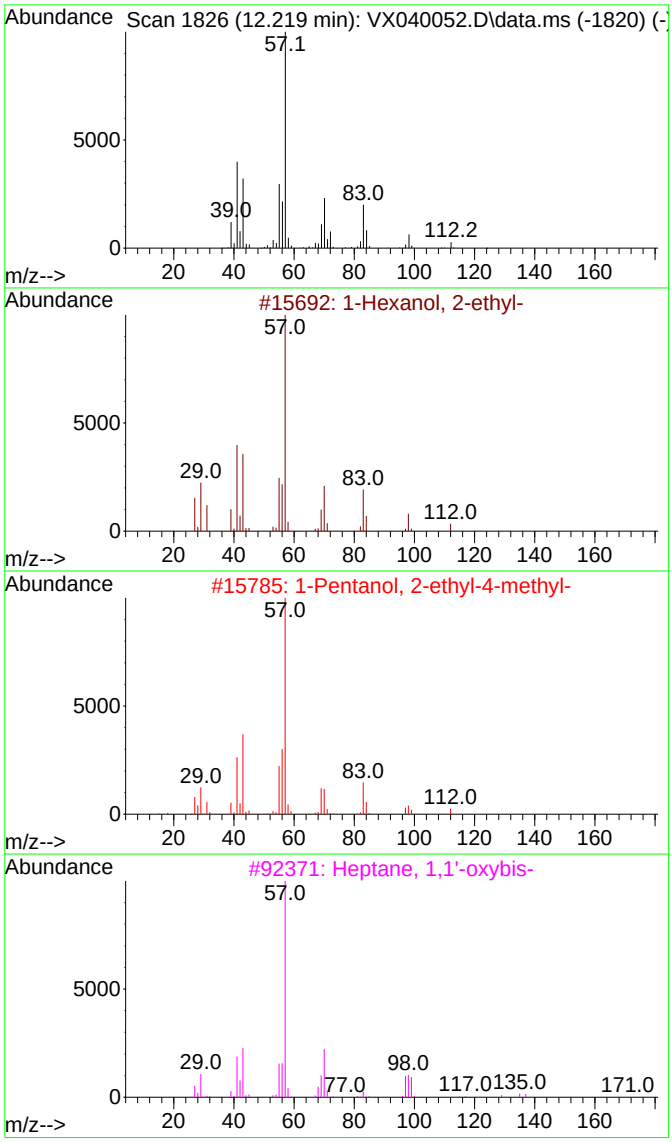
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.M
Quant Title : SW846 8260

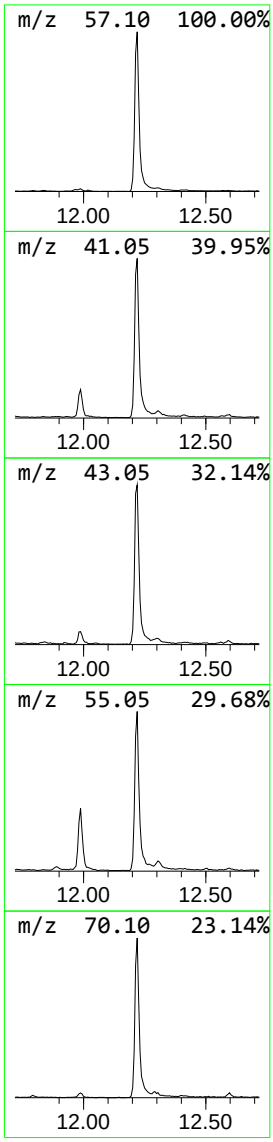
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	90.01 ug/l	937112	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	56
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX013124\
Data File : VX040052.D
Acq On : 31 Jan 2024 17:00
Operator : JC/MD
Sample : P1282-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1241

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X013024W.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	12.0	ug/l	59741	1	5.550	248506	50.0
Acetaldehyde	1.447	333.7	ug/l	1658440	1	5.550	248506	50.0
Ethanol	2.050	10.1	ug/l	50306	1	5.550	248506	50.0
Propanal	2.288	31.1	ug/l	154784	1	5.550	248506	50.0
Butanal	4.227	38.0	ug/l	188971	1	5.550	248506	50.0
1-Butanol	7.208	13.0	ug/l	91755	2	6.757	351868	50.0
4-Heptanol	10.750	19.7	ug/l	184272	3	10.055	467201	50.0
4-Heptanol, 3-m...	11.603	7.9	ug/l	82068	4	12.024	520556	50.0
Butanoic acid, ...	11.683	98.2	ug/l	1022750	4	12.024	520556	50.0
1-Hexanol, 2-et...	12.219	90.0	ug/l	937112	4	12.024	520556	50.0