LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039600.D
Acq On : 03 Jan 2024 14:28
Operator : JC/MD
Sample : P1002-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1212

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: VX039600.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	rVB2	21587	24764	3.23%	0.315%
2	1.239	21	25	31	rBV2	19975	33595	4.38%	0.427%
3	1.355	41	44	49	rBV3	6406	8981	1.17%	0.114%
4	1.453	56	60	67	rBV	29458	36130	4.71%	0.460%
5	1.556	68	77	79	rBV7	8333	21899	2.86%	0.279%
6	2.105	159	167	179	rVB	17144	40746	5.32%	0.518%
7	2.294	191	198	205	rBV	302084	539755	70.41%	6.867%
8	2.379	205	212	231	rVV2	177346	454534	59.30%	5.783%
9	2.581	233	245	257	rVV	71242	199207	25.99%	2.534%
10	2.703	260	265	274	rVB	11595	20427	2.66%	0.260%
11	3.007	299	315	323	rBV2	4479	15391	2.01%	0.196%
12	3.331	360	368	375	rBV3	3104	8666	1.13%	0.110%
13	3.897	449	461	478	rBV	96803	272998	35.61%	3.473%
14	4.227	504	515	523	rBV	49797	135249	17.64%	1.721%
15	4.312	523	529	550	rVB3	20655	72298	9.43%	0.920%
16	4.568	563	571	579	rBV	6676	19895	2.60%	0.253%
17	5.385	695	705	719	rVB	65614	191580	24.99%	2.437%
18	5.550	721	732	745	rBV	96648	277683	36.22%	3.533%
19	5.952	787	798	813	rBV2	77062	209119	27.28%	2.660%
20	6.153	820	831	841	rBV2	8928	28125	3.67%	0.358%
21	6.757	921	930	944	rBV	185542	444647	58.01%	5.657%
22	7.226	1000	1007	1022	rBV	50757	120461	15.71%	1.533%
23	7.476	1042	1048	1060	rVB3	3475	9670	1.26%	0.123%
24	8.647	1234	1240	1250	rBV	396437	620382	80.93%	7.893%
25	8.720	1250	1252	1257	rVV3	4875	7995	1.04%	0.102%
26	8.781	1257	1262	1272	rVB3	5256	11097	1.45%	0.141%
27	9.244	1332	1338	1347	rBV3	8322	17188	2.24%	0.219%
28	10.055	1465	1471	1483	rBV	417217	602283	78.57%	7.662%
29	10.159	1483	1488	1493	rBV3	7854	13447	1.75%	0.171%
30	10.305	1505	1512	1518	rVB2	5040	8952	1.17%	0.114%
31	10.506	1541	1545	1556	rVB	22886	30838	4.02%	0.392%
32	10.604	1556	1561	1565	rBV	5116	9466	1.23%	0.120%
33	10.683	1570	1574	1582	rVB	102438	128465	16.76%	1.634%
34	10.768	1582	1588	1595	rBV2	44263	89731	11.71%	1.142%
35	11.079	1634	1639	1645	rBV	367139	463047	60.41%	5.891%
36	11.128	1645	1647	1654	rVB2	8062	11378	1.48%	0.145%

LSC Area Percent Report

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Acq On : 03 Jan 2024 14:28
Operator : JC/MD
Sample : P1002-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1212

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	11.311	1674	1677	1684	rVV	25203	37684	4.92%	0.479%
38	11.390	1684	1690	1693	rVV3	22058	33605	4.38%	0.428%
39	11.421	1693	1695	1699	rVV	12306	16999	2.22%	0.216%
40	11.481	1702	1705	1713	rVB	5948	8455	1.10%	0.108%
41	11.573	1716	1720	1723	rBV	14930	21846	2.85%	0.278%
42	11.603	1723	1725	1733	rVB4	14189	21773	2.84%	0.277%
43	11.683	1733	1738	1746	rBV	161772	191232	24.95%	2.433%
44	11.756	1746	1750	1754	rBV	6470	8510	1.11%	0.108%
45	11.988	1779	1788	1791	rBV2	403246	766551	100.00%	9.752%
46	12.024	1791	1794	1801	rVV	455313	560499	73.12%	7.131%
47	12.219	1818	1826	1837	rBV	424052	608830	79.42%	7.746%
48	12.305	1837	1840	1854	rVB4	21902	48115	6.28%	0.612%
49	12.561	1878	1882	1885	rBV4	5447	8575	1.12%	0.109%
50	12.768	1911	1916	1918	rBV2	8229	12500	1.63%	0.159%
51	13.140	1971	1977	1988	rBV	42644	60563	7.90%	0.770%
52	13.609	2051	2054	2059	rVB3	6266	8615	1.12%	0.110%
53	13.676	2060	2065	2070	rBV	94810	108918	14.21%	1.386%
54	13.749	2074	2077	2079	rBV3	7007	8850	1.15%	0.113%
55	13.847	2090	2093	2100	rVV5	6551	12383	1.62%	0.158%
56	13.914	2100	2104	2114	rVB4	5520	9923	1.29%	0.126%
57	14.030	2119	2123	2129	rVV	26571	32926	4.30%	0.419%
58	14.133	2135	2140	2146	rBV2	30111	37482	4.89%	0.477%
59	14.268	2158	2162	2166	rVB	18338	21311	2.78%	0.271%
60	14.377	2175	2180	2185	rBV	11138	14130	1.84%	0.180%

Sum of corrected areas: 7860364

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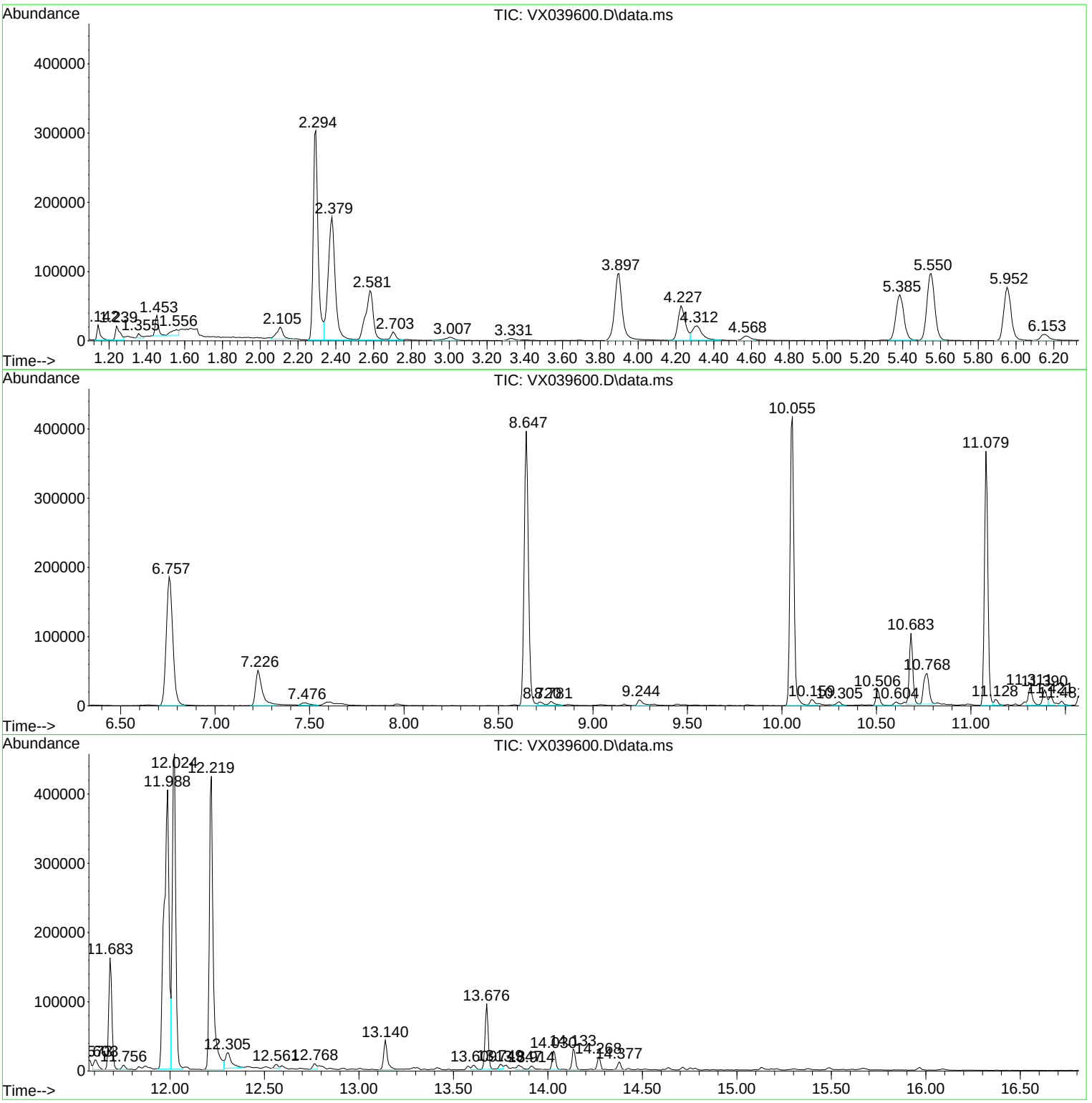
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1212

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



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Data File : VX039600.D
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Quant Title : SW846 8260

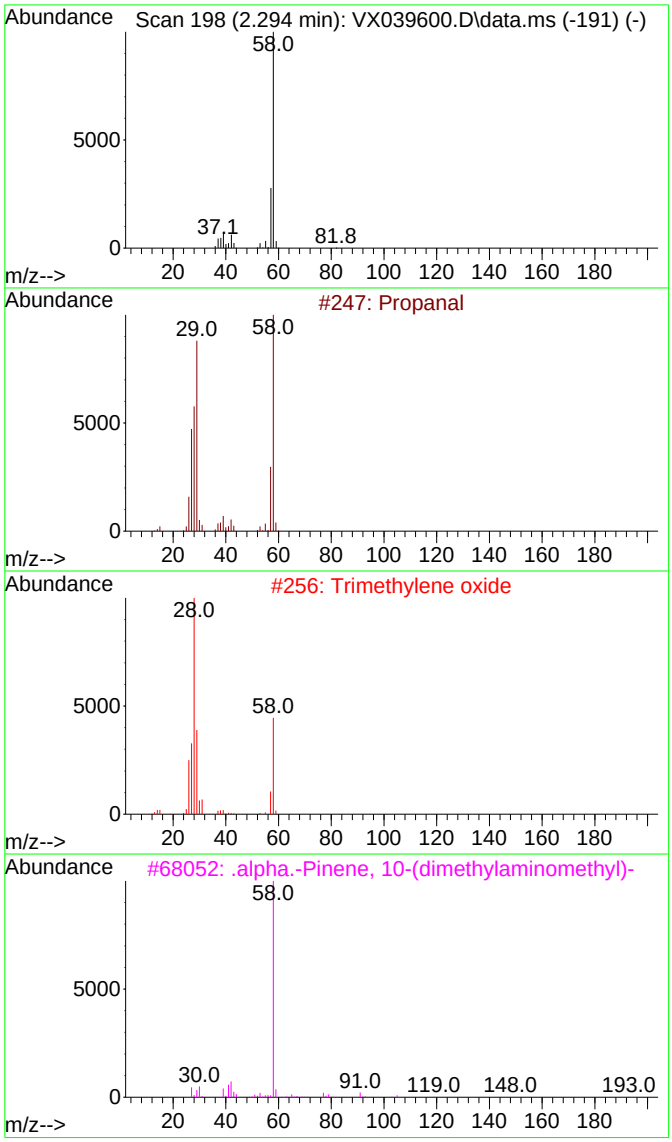
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

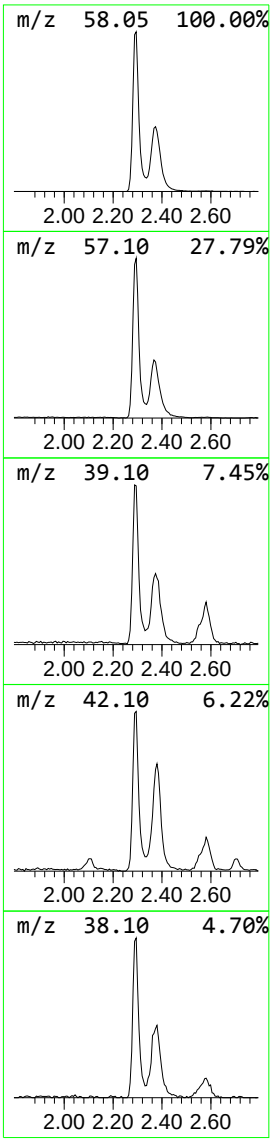
****

Peak Number 1 Propanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.294	97.19 ug/l	539755	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	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7
5	Propylene oxide	58	C3H6O	000075-56-9	5





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039600.D
Acq On : 03 Jan 2024 14:28
Operator : JC/MD
Sample : P1002-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1212

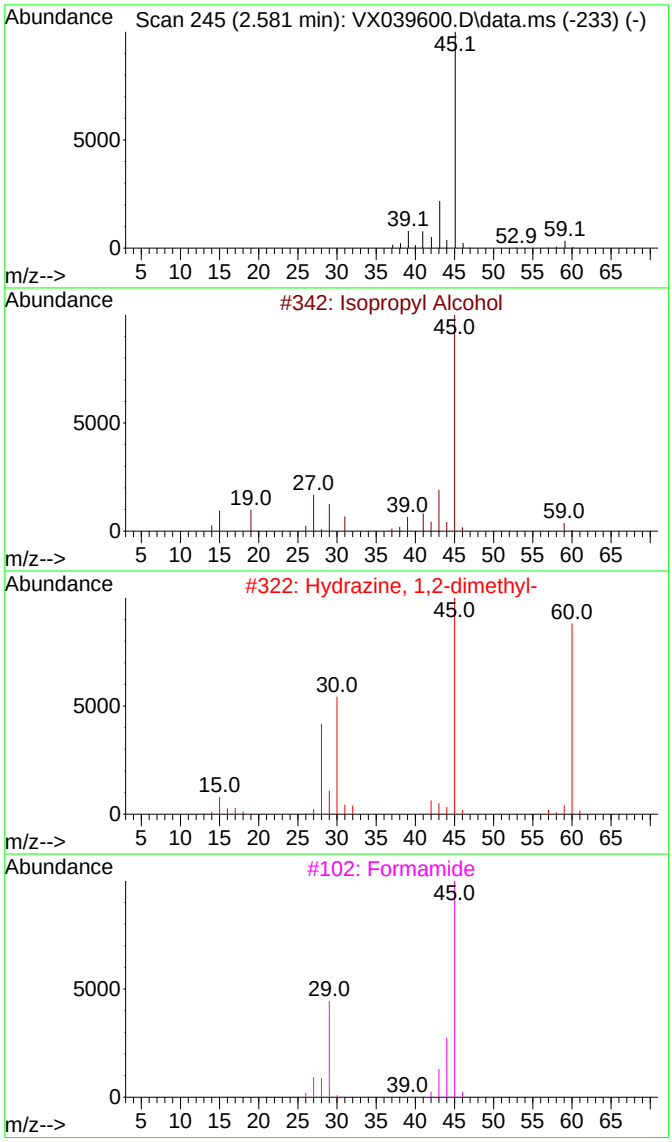
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

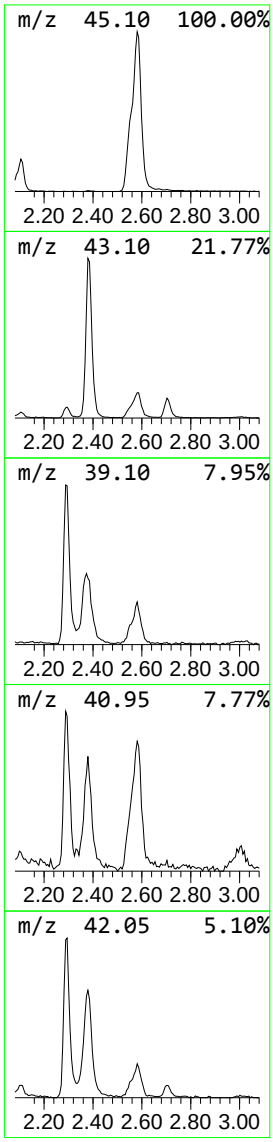
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Isopropyl Alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.581	35.87 ug/l	199207	Pentafluorobenzene	5.550

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	Formamide	45	CH3NO	000075-12-7	5
4	Ethylamine	45	C2H7N	000075-04-7	4
5	2-Propanone, 1-methoxy-	88	C4H8O2	005878-19-3	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039600.D
Acq On : 03 Jan 2024 14:28
Operator : JC/MD
Sample : P1002-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1212

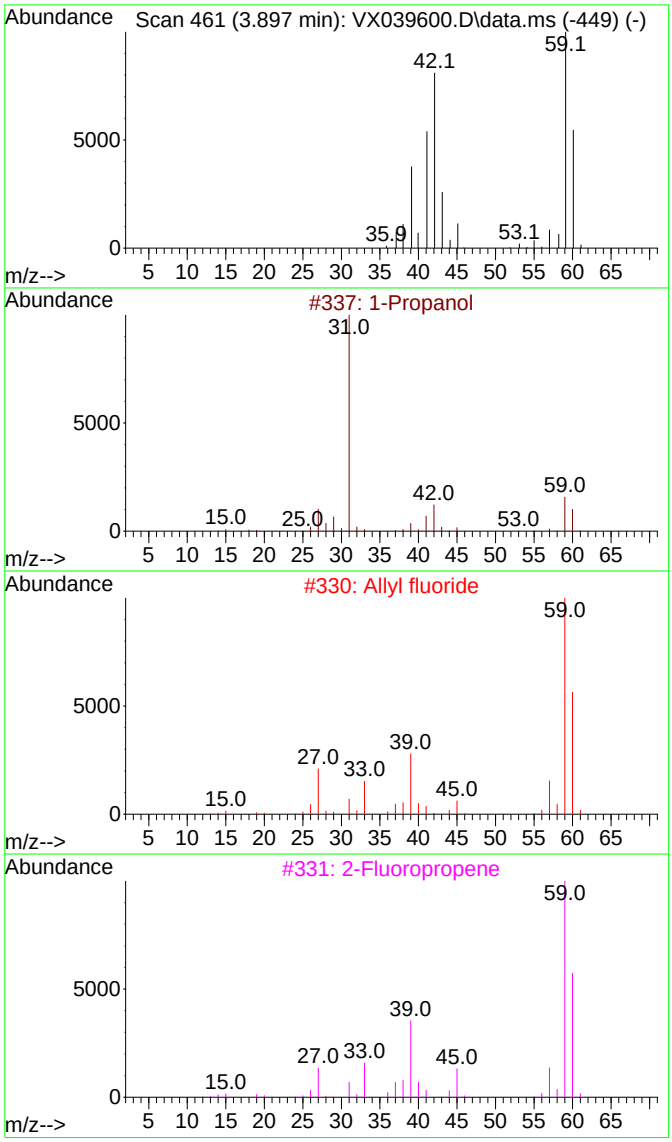
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

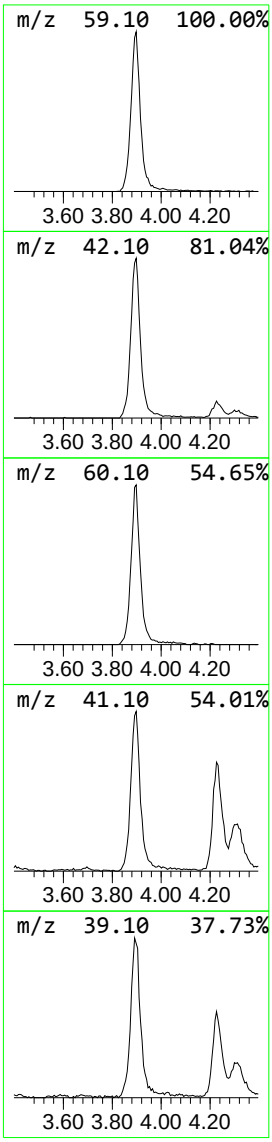
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Propanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.897	49.16 ug/l	272998	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	78
2	Allyl fluoride	60	C3H5F	000818-92-8	47
3	2-Fluoropropene	60	C3H5F	001184-60-7	43
4	2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	17
5	Cyclopropane	42	C3H6	000075-19-4	16





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039600.D
Acq On : 03 Jan 2024 14:28
Operator : JC/MD
Sample : P1002-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1212

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

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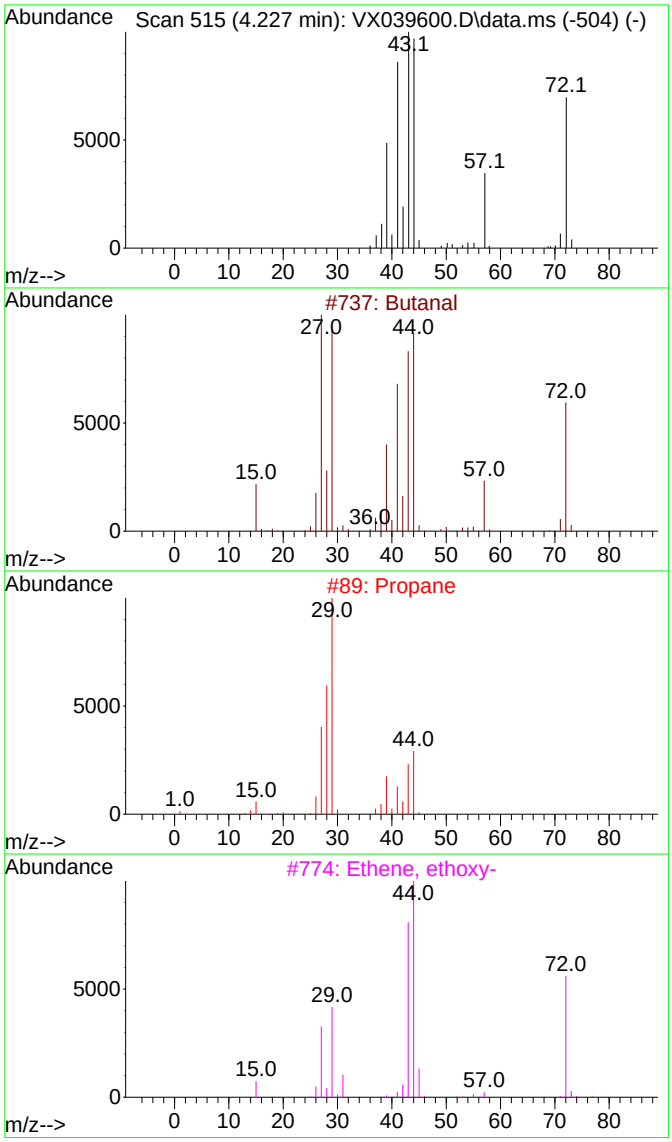
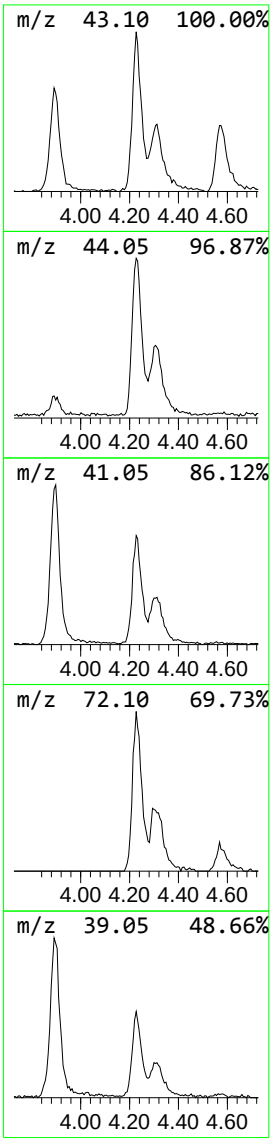
Peak Number 4 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	24.35 ug/l	135249	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Propane	44	C3H8	000074-98-6	59
3	Ethene, ethoxy-	72	C4H8O	000109-92-2	47
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
5	Methacrolein	70	C4H6O	000078-85-3	27





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Operator : JC/MD
Sample : P1002-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1212

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

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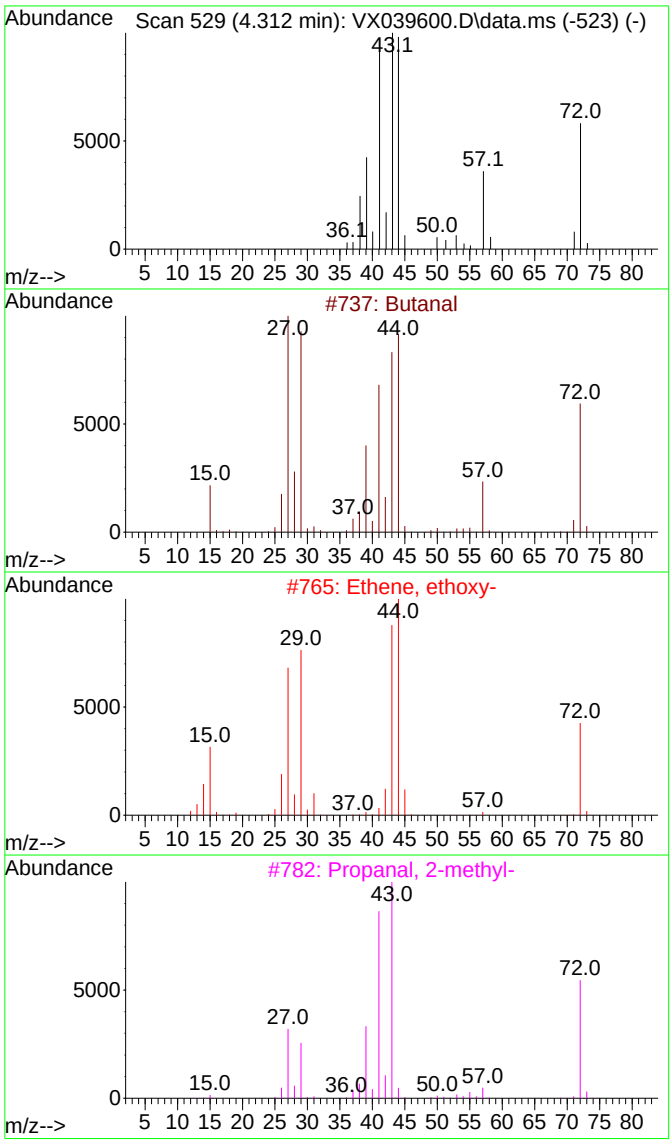
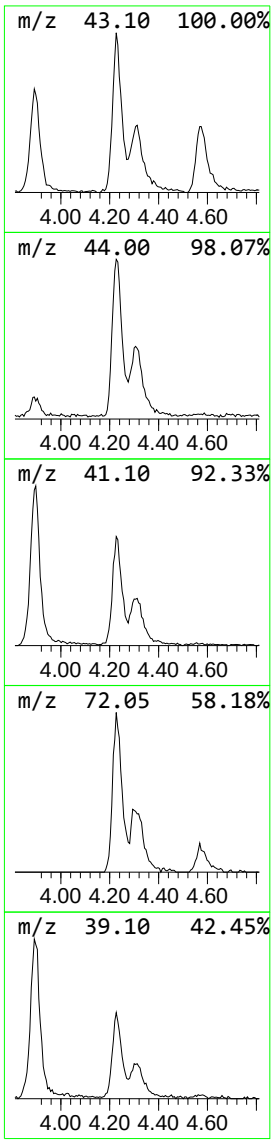
Peak Number 5 unknown4.312 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.312	13.02 ug/l	72298	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	64
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	38
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	35
4	2-Propenoic acid	72	C3H4O2	000079-10-7	9
5	2-Butanone	72	C4H8O	000078-93-3	9





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ALS Vial : 14 Sample Multiplier: 1

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

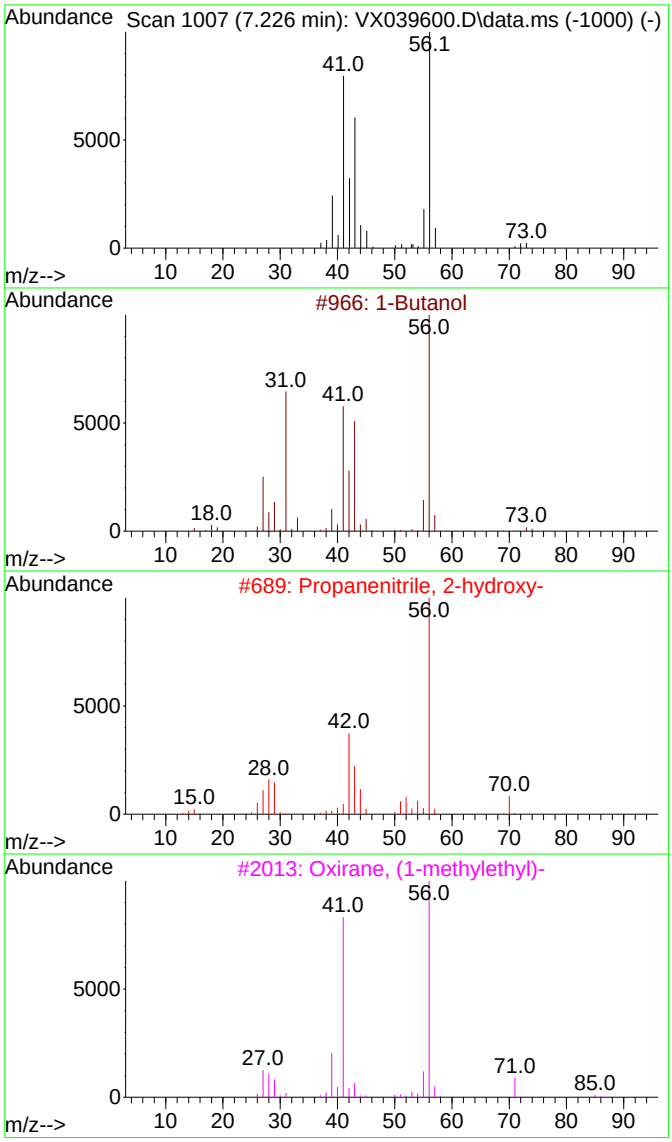
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

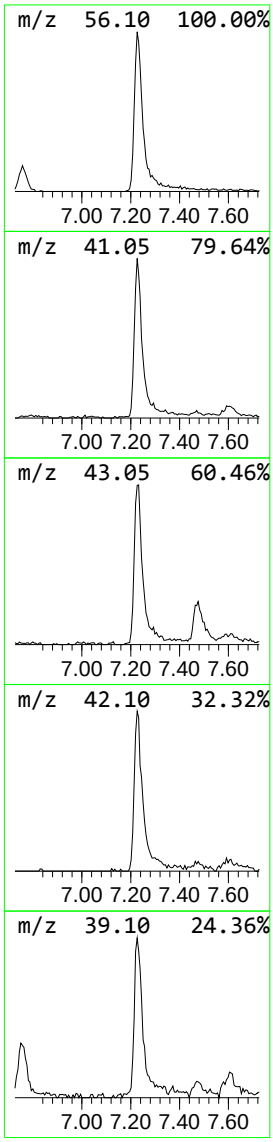
****

Peak Number 6 1-Butanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.226	13.55 ug/l	120461	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	64
2	Propanenitrile, 2-hydroxy-	71	C3H5NO	000078-97-7	50
3	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	38
4	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	38
5	.alpha.-Amino-.gamma.-butyrolactone	101	C4H7NO2	001192-20-7	10





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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1212

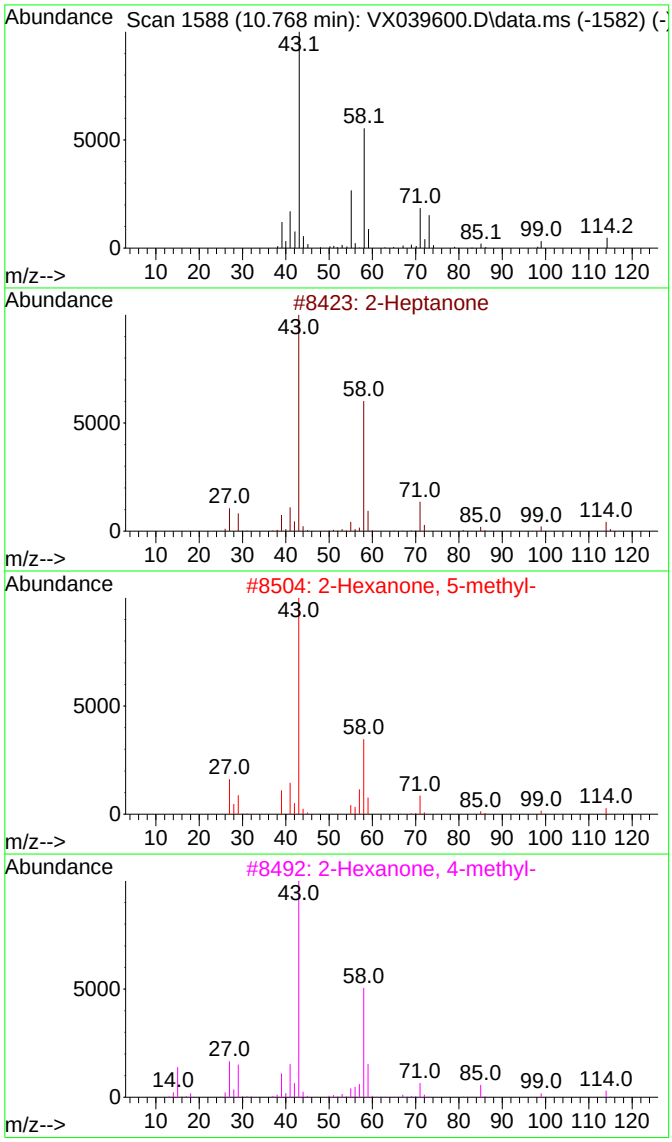
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

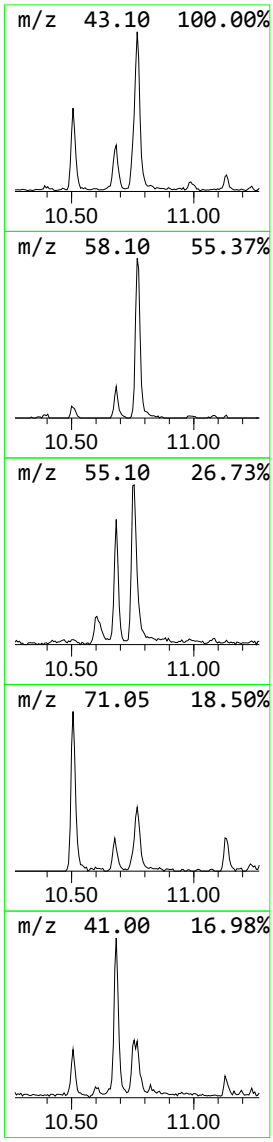
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Heptanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.768	7.45 ug/l	89731	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone	114	C7H14O	000110-43-0	83
2	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	64
3	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	53
4	Butanimidamide	86	C4H10N2	000107-90-4	38
5	6-Dimethylamino-4-ketohexanoic a...	187	C9H17NO3	1000353-25-7	38





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Data File : VX039600.D
Acq On : 03 Jan 2024 14:28
Operator : JC/MD
Sample : P1002-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1212

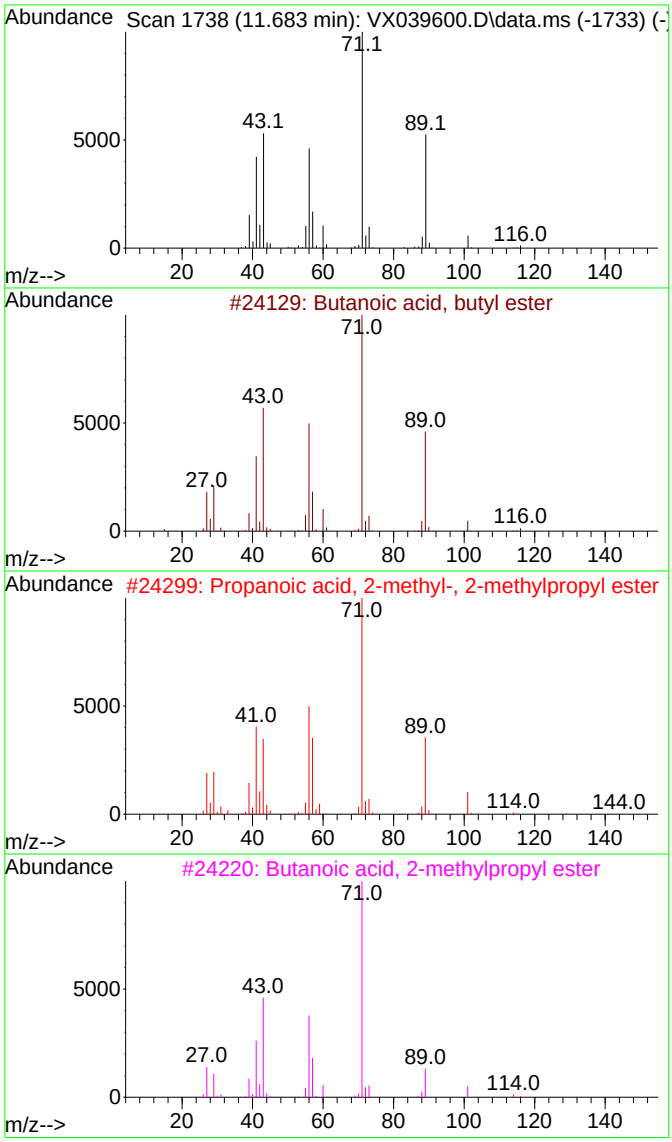
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

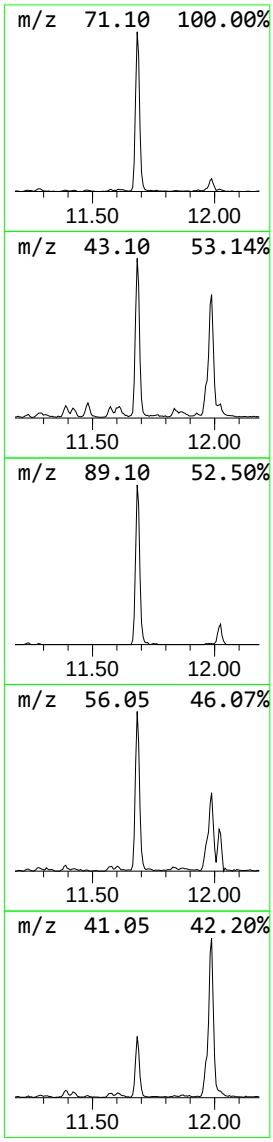
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Butanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	17.06 ug/l	191232	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	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	72
3	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
4	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
5	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039600.D
Acq On : 03 Jan 2024 14:28
Operator : JC/MD
Sample : P1002-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1212

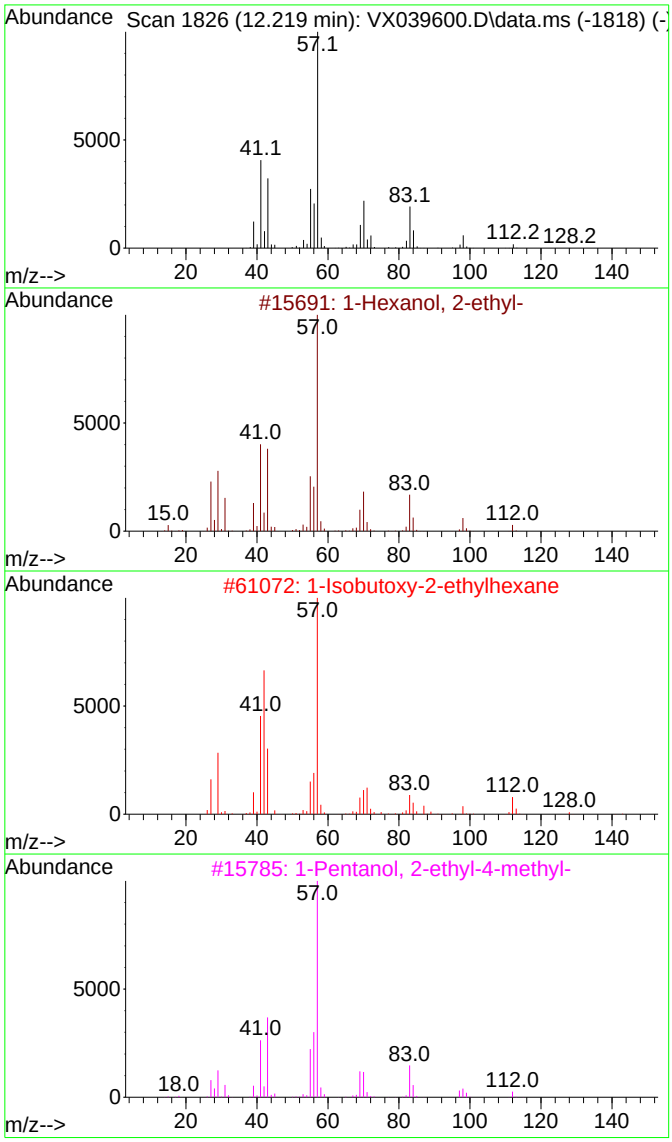
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

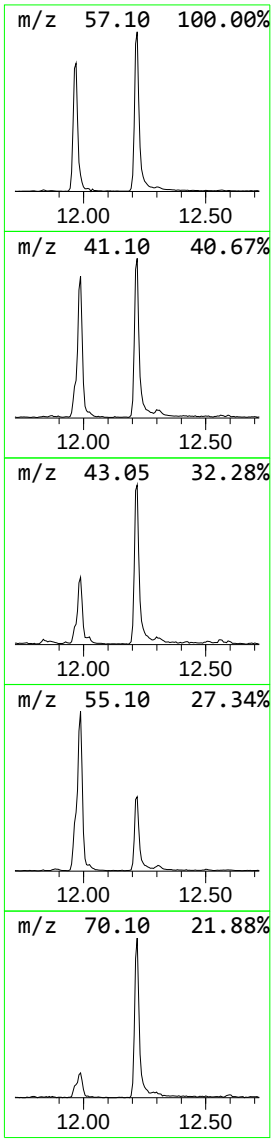
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	54.31 ug/l	608830	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	78
2	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	74
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039600.D
Acq On : 03 Jan 2024 14:28
Operator : JC/MD
Sample : P1002-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1212

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

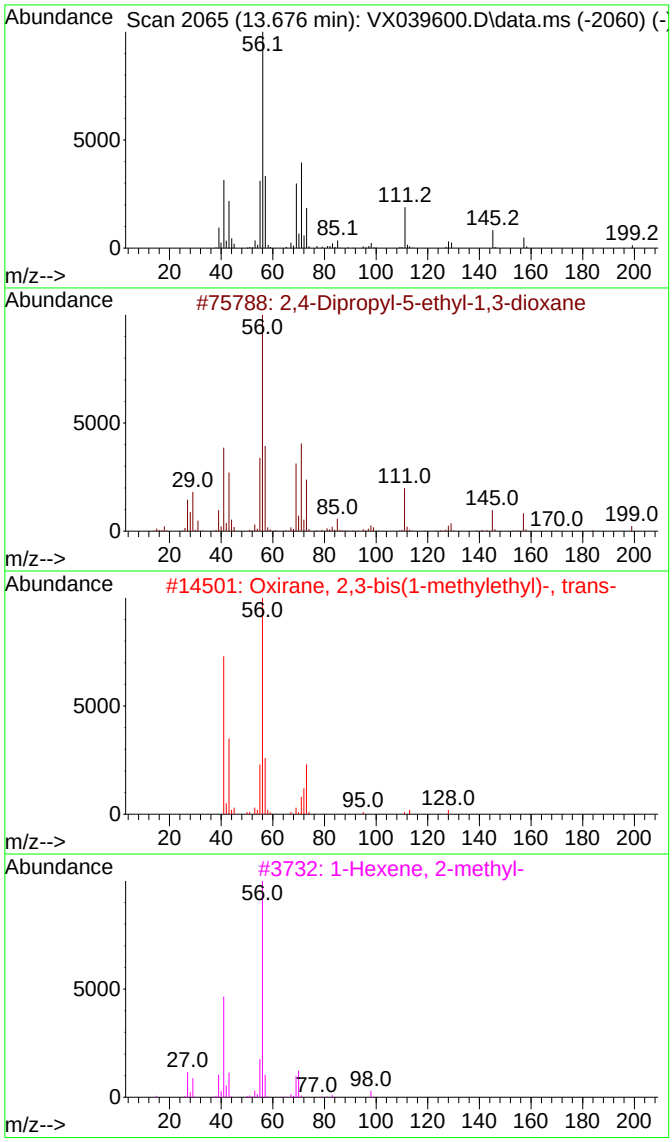
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

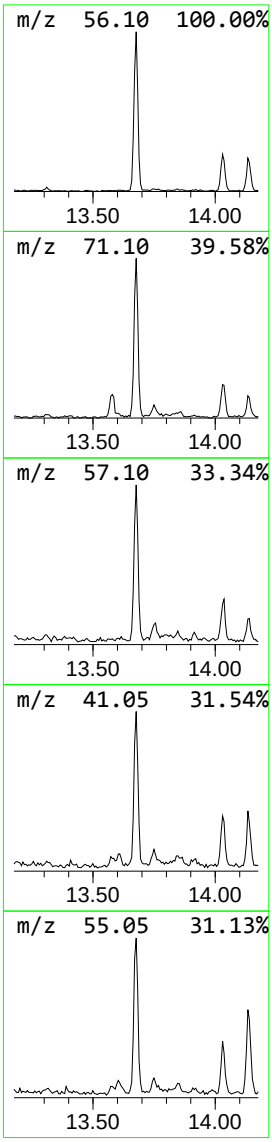
****

Peak Number 10 unknown13.676 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	9.72 ug/l	108918	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	47
2	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	25
3	1-Hexene, 2-methyl-	98	C7H14	006094-02-6	25
4	1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	25
5	1-Octene, 2-methyl-	126	C9H18	004588-18-5	23





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039600.D
Acq On : 03 Jan 2024 14:28
Operator : JC/MD
Sample : P1002-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1212

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
Propanal	2.294	97.2	ug/l	539755	1	5.550	277683	50.0
Isopropyl Alcohol	2.581	35.9	ug/l	199207	1	5.550	277683	50.0
1-Propanol	3.897	49.2	ug/l	272998	1	5.550	277683	50.0
Butanal	4.227	24.4	ug/l	135249	1	5.550	277683	50.0
unknown4.312	4.312	13.0	ug/l	72298	1	5.550	277683	50.0
1-Butanol	7.226	13.6	ug/l	120461	2	6.757	444647	50.0
2-Heptanone	10.768	7.5	ug/l	89731	3	10.055	602283	50.0
Butanoic acid, ...	11.683	17.1	ug/l	191232	4	12.024	560499	50.0
1-Hexanol, 2-et...	12.219	54.3	ug/l	608830	4	12.024	560499	50.0
unknown13.676	13.676	9.7	ug/l	108918	4	12.024	560499	50.0