LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039606.D
Acq On : 03 Jan 2024 16:44
Operator : JC/MD
Sample : P1002-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1218

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: VX039606.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	24	27	41	rBV	11512264	14177028	100.00%	38.035%
2	2.050	151	158	171	rBV	620968	1019570	7.19%	2.735%
3	2.373	204	211	218	rBV	719957	1161670	8.19%	3.117%
4	4.227	504	515	530	rBV	307138	819414	5.78%	2.198%
5	4.550	558	568	588	rBV	171435	488338	3.44%	1.310%
6	5.385	693	705	722	rBV2	73836	213286	1.50%	0.572%
7	5.550	722	732	749	rVB	104380	292112	2.06%	0.784%
8	5.952	788	798	806	rBV2	81520	216558	1.53%	0.581%
9	6.098	816	822	835	rVB	73633	194635	1.37%	0.522%
10	6.757	921	930	945	rVB	196031	473196	3.34%	1.270%
11	7.196	991	1002	1014	rBV	184201	398495	2.81%	1.069%
12	7.452	1029	1044	1051	rBV	119558	241448	1.70%	0.648%
13	8.647	1234	1240	1246	rBV	432109	671337	4.74%	1.801%
14	8.714	1246	1251	1256	rBV	171027	275015	1.94%	0.738%
15	10.055	1461	1471	1476	rBV	497723	752843	5.31%	2.020%
16	10.152	1482	1487	1491	rBV	182198	245550	1.73%	0.659%
17	10.299	1506	1511	1520	rVB	326357	442594	3.12%	1.187%
18	10.500	1540	1544	1551	rVB	199157	251905	1.78%	0.676%
19	10.640	1562	1567	1570	rBV	160447	217838	1.54%	0.584%
20	10.677	1570	1573	1580	rVB	673333	812892	5.73%	2.181%
21	10.750	1580	1585	1593	rBV3	322309	488778	3.45%	1.311%
22	11.079	1633	1639	1643	rBV	470549	604134	4.26%	1.621%
23	11.128	1643	1647	1652	rVB	352851	416721	2.94%	1.118%
24	11.567	1712	1719	1722	rBV2	234409	376570	2.66%	1.010%
25	11.603	1722	1725	1731	rVV3	192338	308133	2.17%	0.827%
26	11.683	1734	1738	1744	rVB	664053	745094	5.26%	1.999%
27	11.750	1745	1749	1754	rBV2	139388	194687	1.37%	0.522%
28	12.018	1789	1793	1801	rVB2	576148	814446	5.74%	2.185%
29	12.219	1821	1826	1836	rBV	6787686	8330536	58.76%	22.350%
30	12.304	1836	1840	1853	rVB3	247773	418792	2.95%	1.124%
31	12.560	1878	1882	1886	rBV3	124067	169536	1.20%	0.455%
32	13.676	2060	2065	2070	rBV2	120445	169772	1.20%	0.455%
33	13.749	2073	2077	2078	rBV	176961	186433	1.32%	0.500%
34	13.774	2078	2081	2085	rVB	269794	345287	2.44%	0.926%
35	13.841	2090	2092	2100	rVV2	116706	178942	1.26%	0.480%
36	13.914	2100	2104	2110	rVB	120519	159724	1.13%	0.429%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039606.D
Acq On : 03 Jan 2024 16:44
Operator : JC/MD
Sample : P1002-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1218

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

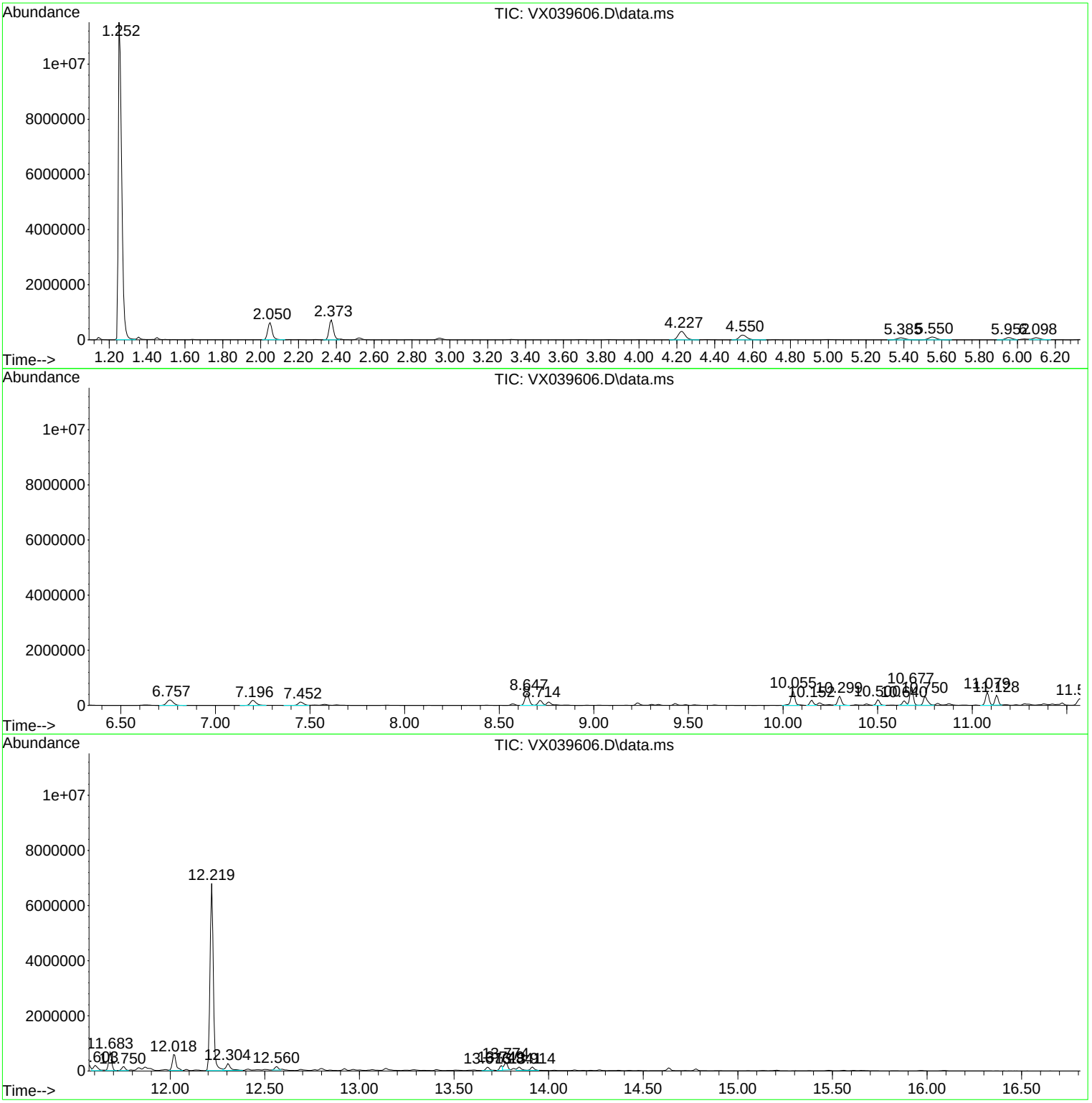
Sum of corrected areas: 37273309

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039606.D
Acq On : 03 Jan 2024 16:44
Operator : JC/MD
Sample : P1002-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1218

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 : VX039606.D
Acq On : 03 Jan 2024 16:44
Operator : JC/MD
Sample : P1002-10
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Instrument :
MSVOA_X
ClientSampleId :
1218

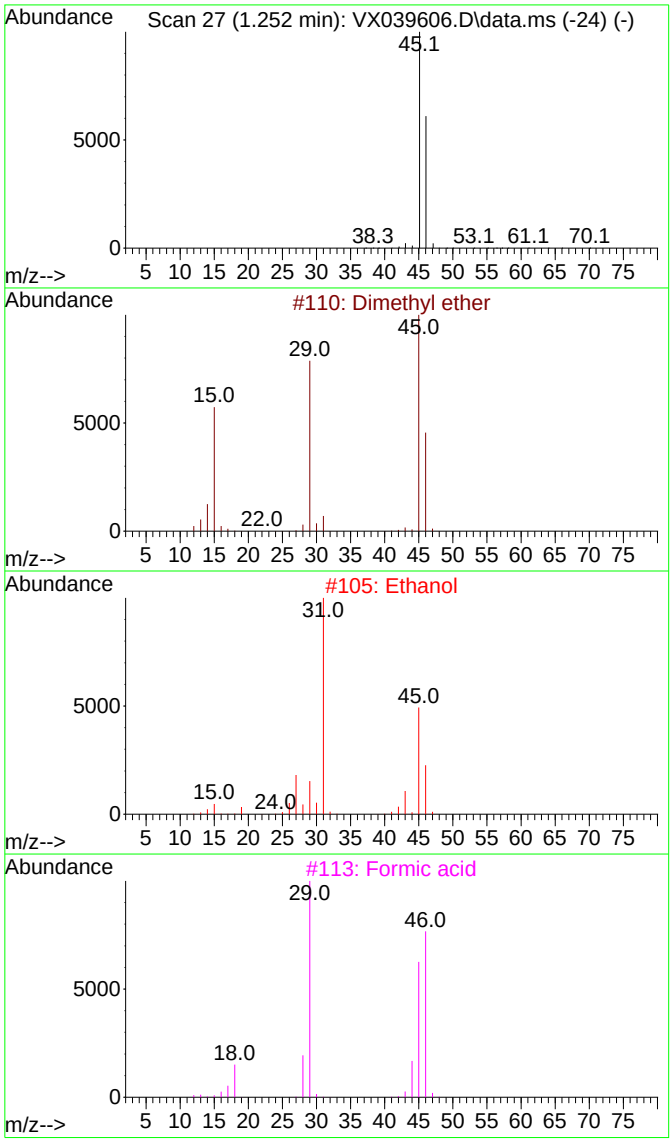
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

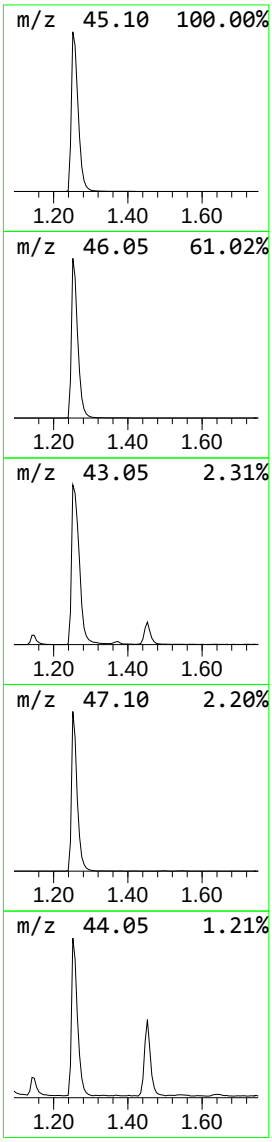
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	2426.64 ug/l	14177000	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl ether	46	C2H6O	000115-10-6	90
2	Ethanol	46	C2H6O	000064-17-5	7
3	Formic acid	46	CH2O2	000064-18-6	7
4	Hydrazine, methyl-	46	CH6N2	000060-34-4	4
5	Ethene, fluoro-	46	C2H3F	000075-02-5	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039606.D
Acq On : 03 Jan 2024 16:44
Operator : JC/MD
Sample : P1002-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1218

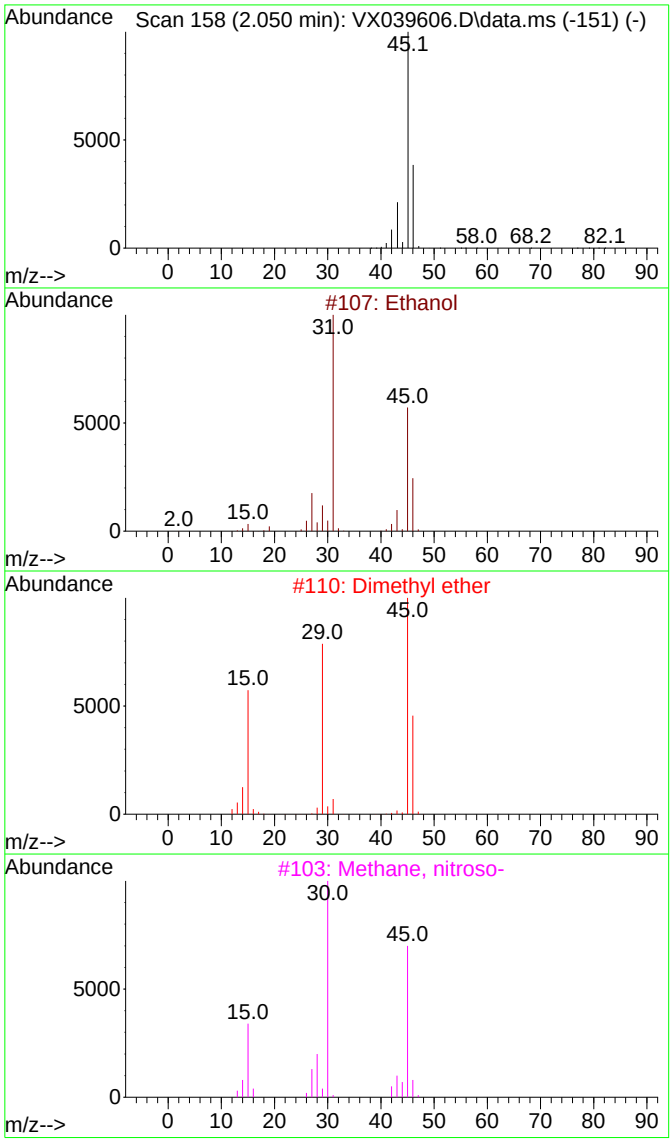
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

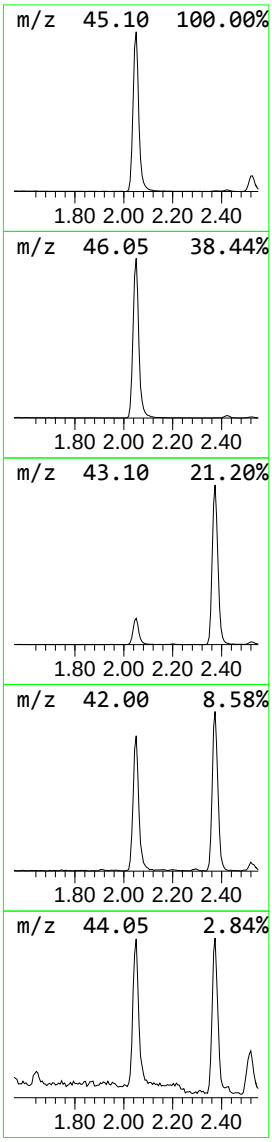
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.050	174.52 ug/l	1019570	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	L-Lactic acid	90	C3H6O3	000079-33-4	2





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039606.D
Acq On : 03 Jan 2024 16:44
Operator : JC/MD
Sample : P1002-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1218

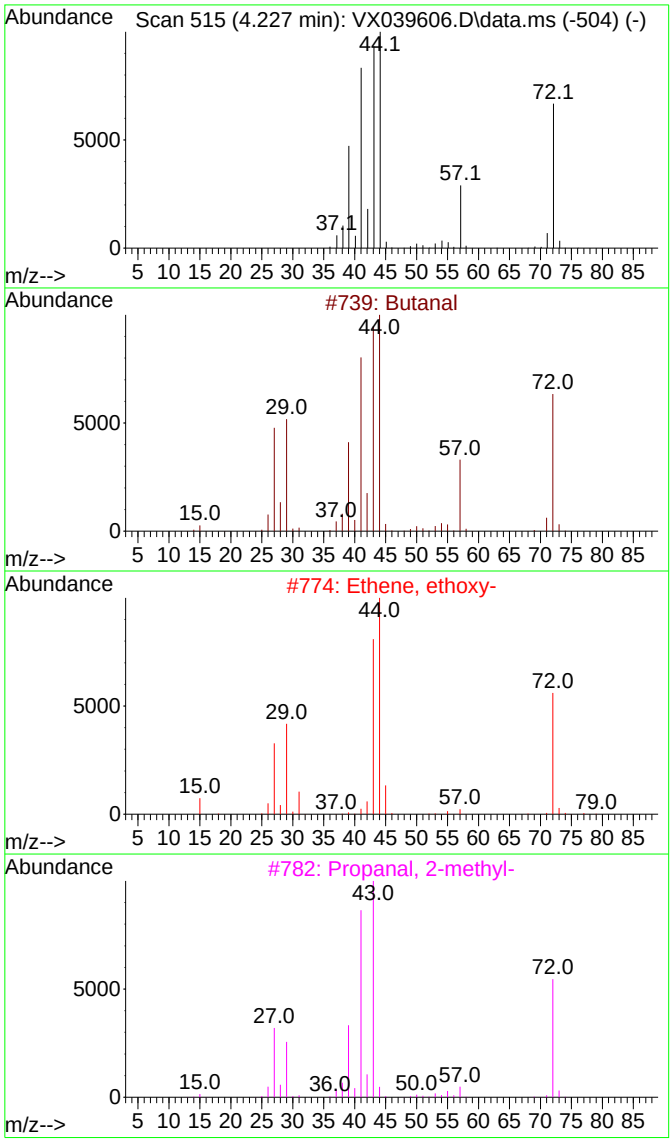
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

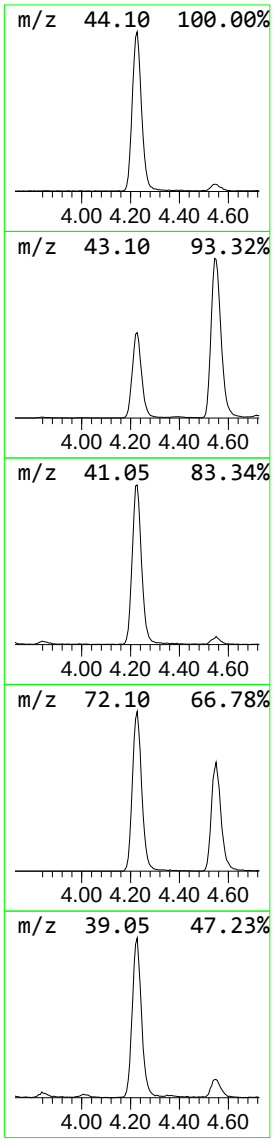
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	140.26 ug/l	819414	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	43
4	2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	32
5	Cyclopropyl carbinol	72	C4H8O	002516-33-8	23





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039606.D
Acq On : 03 Jan 2024 16:44
Operator : JC/MD
Sample : P1002-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1218

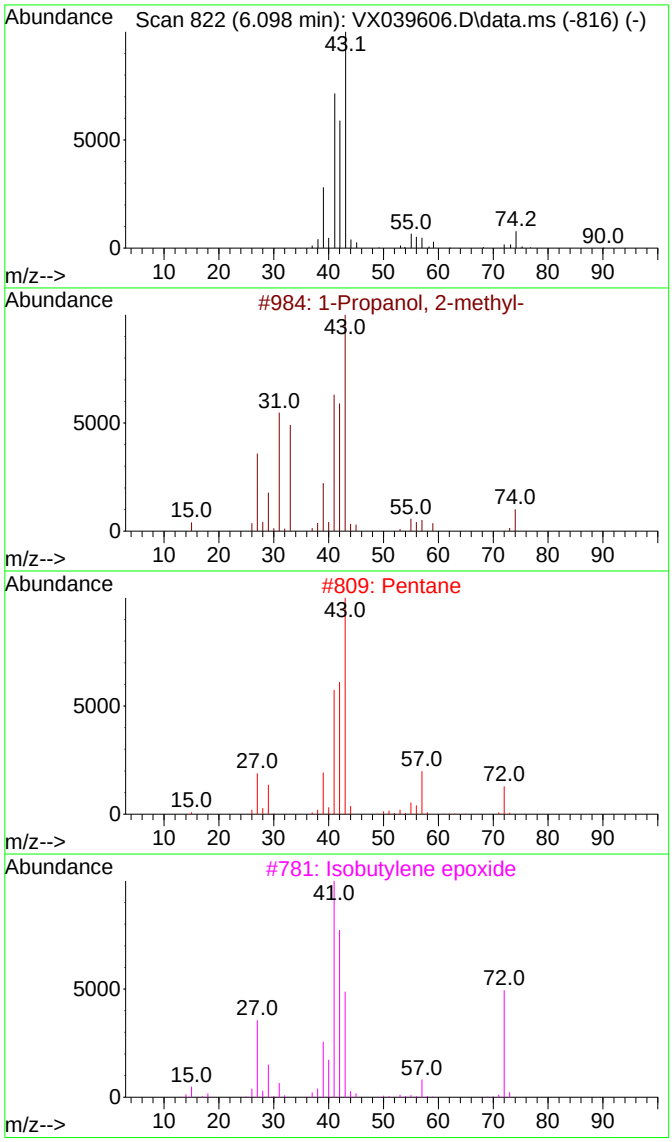
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

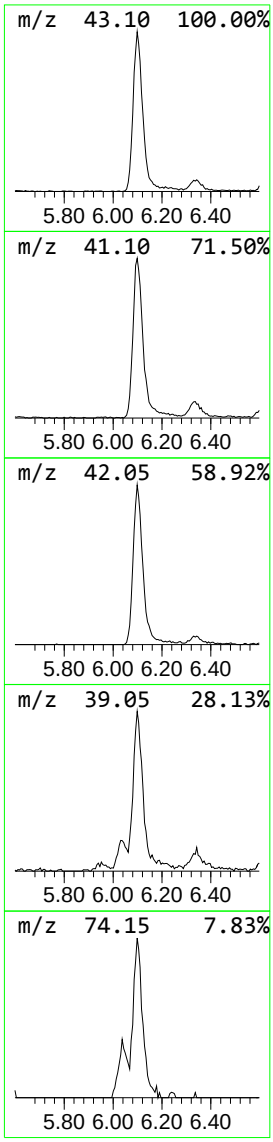
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1-Propanol, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.098	33.32 ug/l	194635	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	91
2	Pentane	72	C5H12	000109-66-0	45
3	Isobutylene epoxide	72	C4H8O	000558-30-5	43
4	Oxirane, ethyl-	72	C4H8O	000106-88-7	17
5	Propanal, 2-methyl-	72	C4H8O	000078-84-2	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039606.D
Acq On : 03 Jan 2024 16:44
Operator : JC/MD
Sample : P1002-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1218

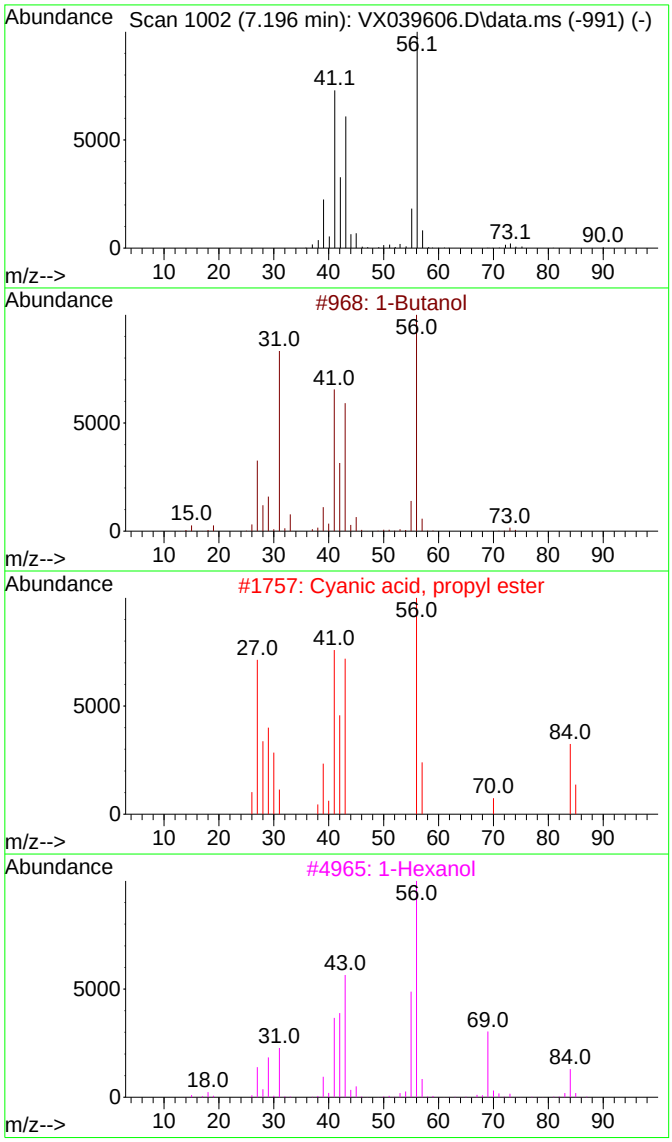
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

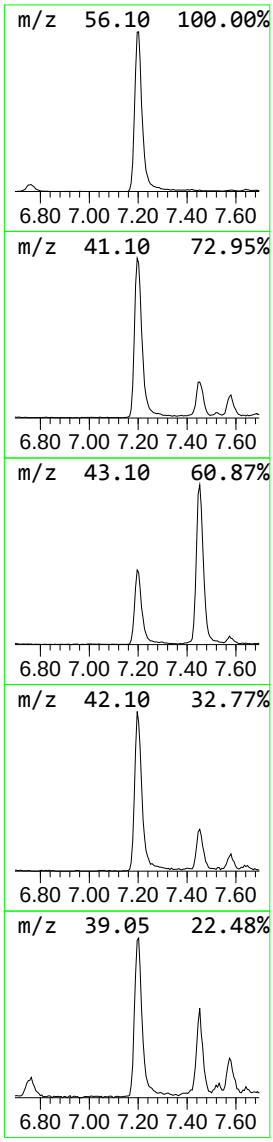
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.196	42.11 ug/l	398495	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	86
2	Cyanic acid, propyl ester	85	C4H7NO	001768-36-1	45
3	1-Hexanol	102	C6H14O	000111-27-3	40
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	38
5	Hydroperoxide, hexyl	118	C6H14O2	004312-76-9	23





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039606.D
Acq On : 03 Jan 2024 16:44
Operator : JC/MD
Sample : P1002-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1218

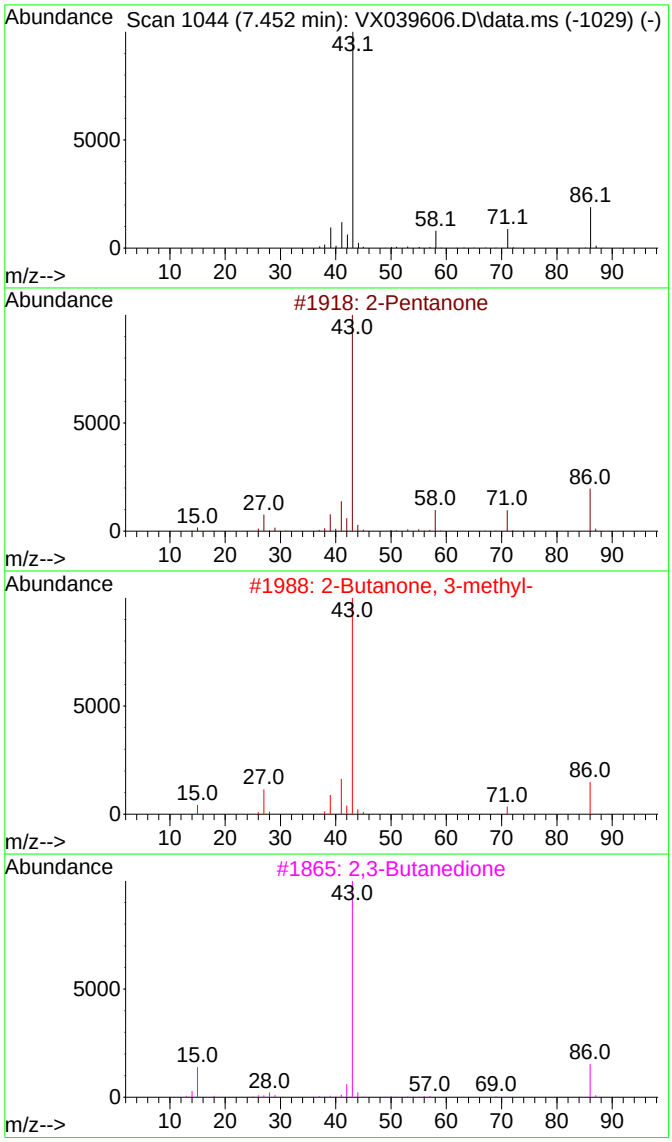
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

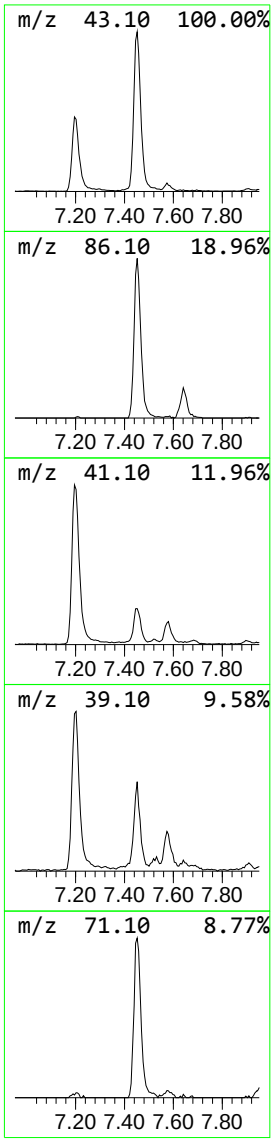
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Pentanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.452	25.51 ug/l	241448	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	91
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	59
3	2,3-Butanedione	86	C4H6O2	000431-03-8	53
4	3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	36
5	Butane	58	C4H10	000106-97-8	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039606.D
Acq On : 03 Jan 2024 16:44
Operator : JC/MD
Sample : P1002-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1218

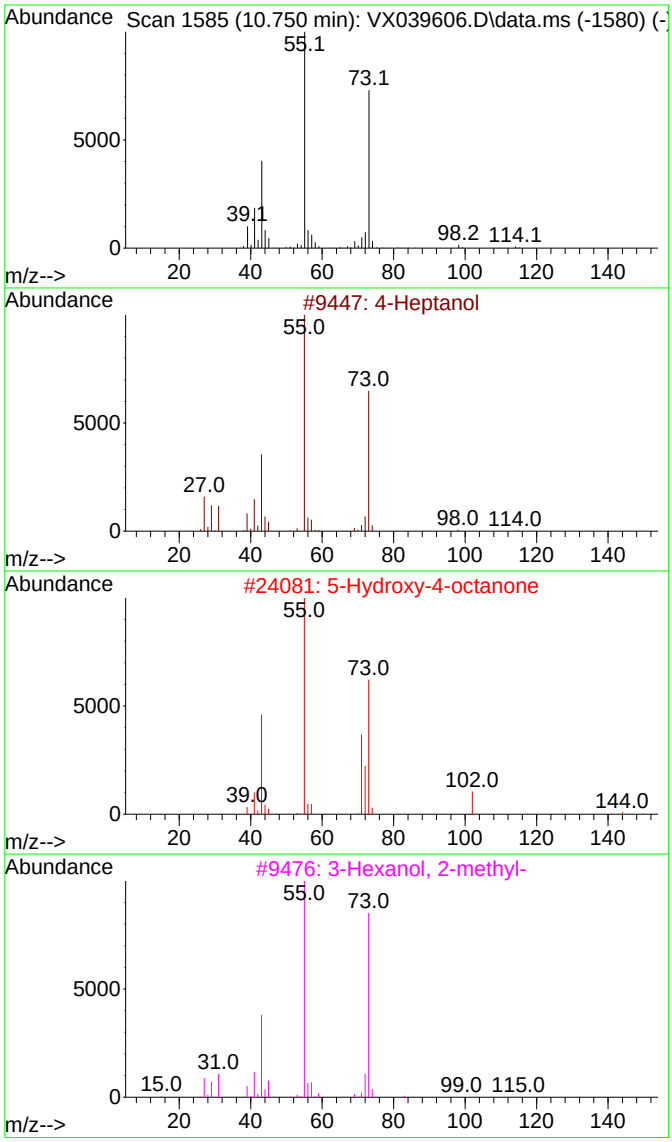
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

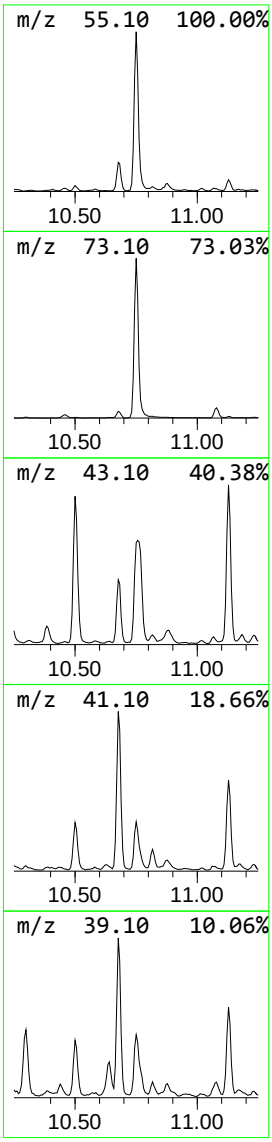
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 4-Heptanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.750	32.46 ug/l	488778	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	59
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	45
4	4,5-Octanediol	146	C8H18O2	022607-10-9	38
5	Oxalic acid, cyclobutyl hexyl ester	228	C12H20O4	1000309-69-7	38





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Data File : VX039606.D
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Operator : JC/MD
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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1218

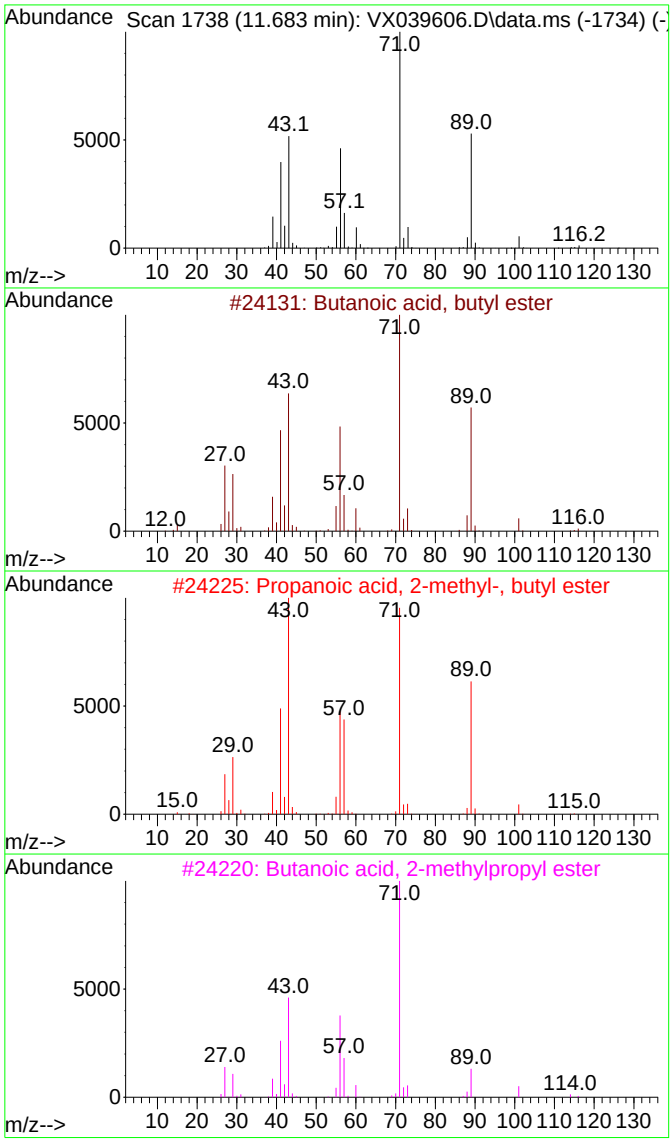
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

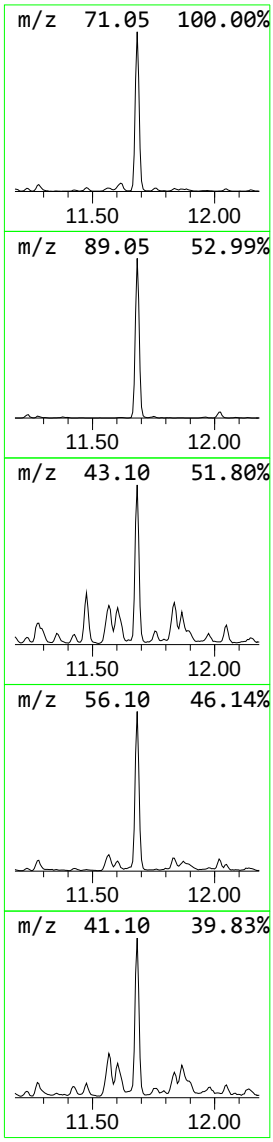
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Butanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	45.74 ug/l	745094	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-, butyl...	144	C8H16O2	000097-87-0	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, hexyl ester	172	C10H20O2	002639-63-6	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039606.D
Acq On : 03 Jan 2024 16:44
Operator : JC/MD
Sample : P1002-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1218

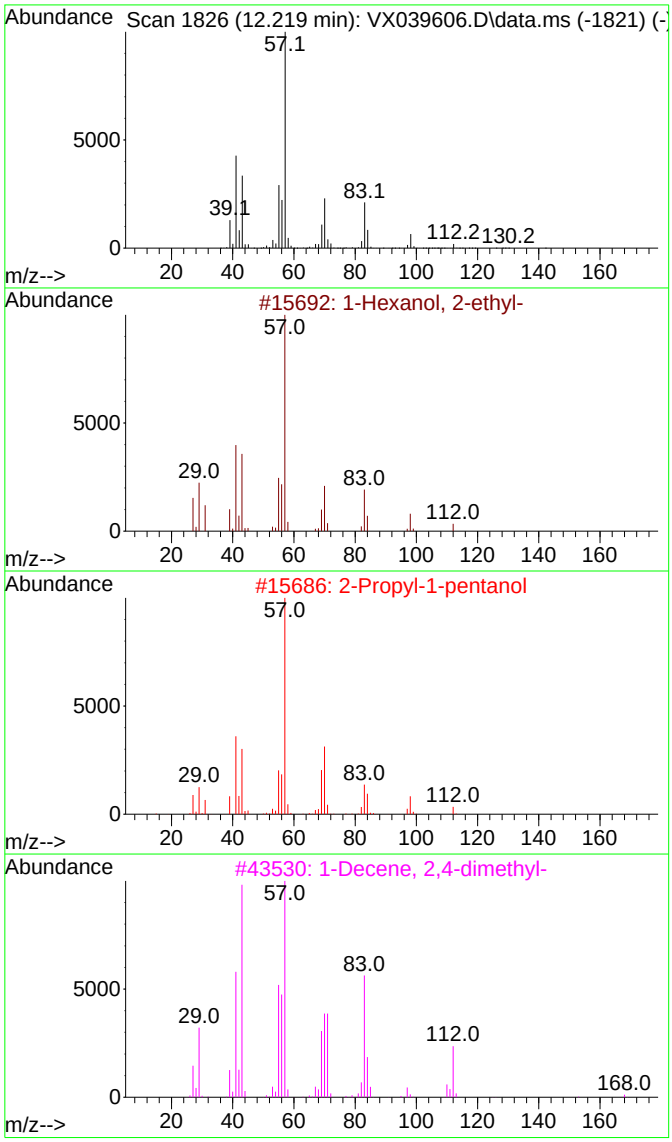
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

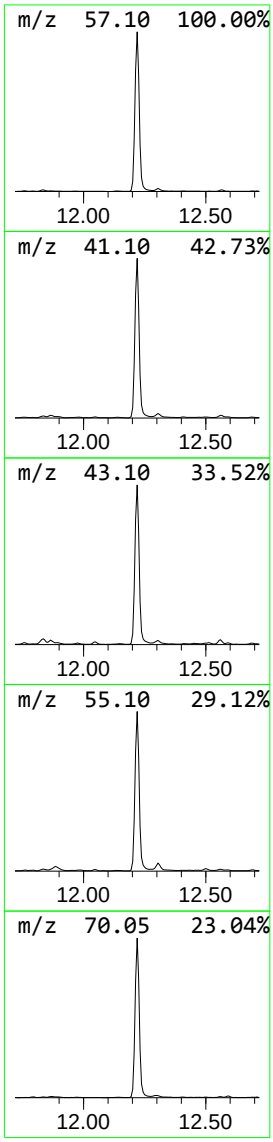
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	511.42 ug/l	8330540	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	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
3	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	47
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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039606.D
Acq On : 03 Jan 2024 16:44
Operator : JC/MD
Sample : P1002-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1218

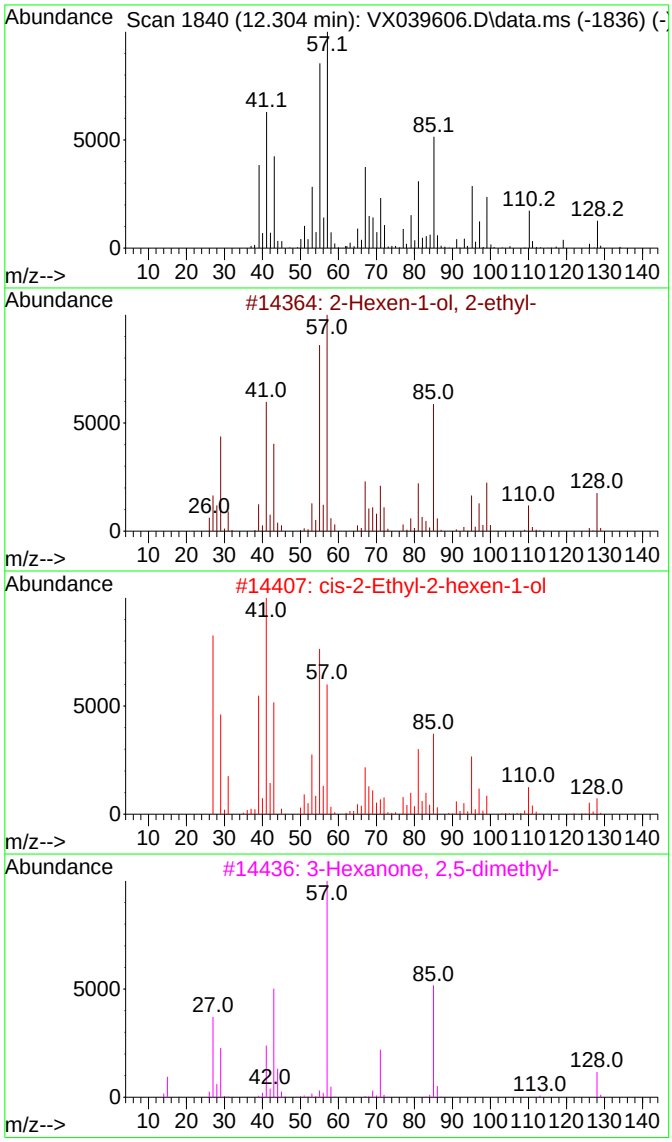
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

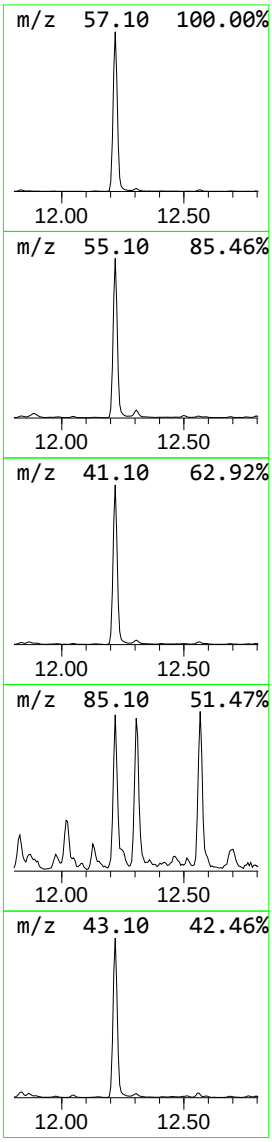
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2-Hexen-1-ol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.304	25.71 ug/l	418792	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexen-1-ol, 2-ethyl-	128	C8H16O	050639-00-4	94
2	cis-2-Ethyl-2-hexen-1-ol	128	C8H16O	1000139-52-4	47
3	3-Hexanone, 2,5-dimethyl-	128	C8H16O	001888-57-9	45
4	3-Heptanone, 2-methyl-	128	C8H16O	013019-20-0	38
5	Pentane, 3-ethyl-2,3-dimethyl-	128	C9H20	016747-33-4	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039606.D
Acq On : 03 Jan 2024 16:44
Operator : JC/MD
Sample : P1002-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1218

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	2426.6	ug/l	14177000	1	5.550	292112	50.0
Ethanol	2.050	174.5	ug/l	1019570	1	5.550	292112	50.0
Butanal	4.227	140.3	ug/l	819414	1	5.550	292112	50.0
1-Propanol, 2-m...	6.098	33.3	ug/l	194635	1	5.550	292112	50.0
1-Butanol	7.196	42.1	ug/l	398495	2	6.763	473196	50.0
2-Pentanone	7.452	25.5	ug/l	241448	2	6.763	473196	50.0
4-Heptanol	10.750	32.5	ug/l	488778	3	10.055	752843	50.0
Butanoic acid, ...	11.683	45.7	ug/l	745094	4	12.024	814446	50.0
1-Hexanol, 2-et...	12.219	511.4	ug/l	8330540	4	12.024	814446	50.0
2-Hexen-1-ol, 2...	12.304	25.7	ug/l	418792	4	12.024	814446	50.0