LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
Data File : VX031129.D
Acq On : 06 Sep 2022 15:39
Operator : JC/MD
Sample : N4489-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1504

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\82X090122W.M
Title : SW846 8260

Signal : TIC: VX031129.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.453	56	60	71	rBV	262212	362490	3.08%	0.873%
2	2.166	155	177	188	rBV3	124006	985648	8.37%	2.373%
3	2.300	194	199	207	rVB	243631	466662	3.96%	1.123%
4	2.398	207	215	236	rVB	4531987	11773399	100.00%	28.343%
5	2.617	236	251	254	rBV	673360	3078723	26.15%	7.412%
6	3.946	444	469	470	rBV	2160326	7614157	64.67%	18.330%
7	4.690	580	591	620	rVB	203771	1045590	8.88%	2.517%
8	5.275	671	687	701	rBV	143178	519518	4.41%	1.251%
9	5.428	703	712	725	rVB2	104632	327043	2.78%	0.787%
10	5.574	725	736	753	rVB	204091	577669	4.91%	1.391%
11	5.982	794	803	825	rVB	111273	332769	2.83%	0.801%
12	6.775	924	933	944	rVB	281487	686277	5.83%	1.652%
13	7.318	1013	1022	1028	rBV2	93110	225627	1.92%	0.543%
14	7.818	1098	1104	1119	rVB	94554	182747	1.55%	0.440%
15	8.653	1235	1241	1248	rVB	656765	1008687	8.57%	2.428%
16	8.823	1256	1269	1291	rVV	186044	674534	5.73%	1.624%
17	9.006	1293	1299	1309	rVB	1487366	2577833	21.90%	6.206%
18	9.171	1320	1326	1335	rVB	319339	543856	4.62%	1.309%
19	9.275	1338	1343	1358	rBV	739552	1510545	12.83%	3.636%
20	9.494	1373	1379	1386	rVB	1207100	1775867	15.08%	4.275%
21	10.055	1466	1471	1480	rVB	523562	746653	6.34%	1.797%
22	10.171	1485	1490	1508	rBV	1912953	2703446	22.96%	6.508%
23	11.085	1634	1640	1646	rBV	562300	703650	5.98%	1.694%
24	12.024	1789	1794	1803	rVB	597512	783125	6.65%	1.885%
25	12.225	1822	1827	1835	rBV2	184819	332936	2.83%	0.801%

Sum of corrected areas: 41539451

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Instrument :
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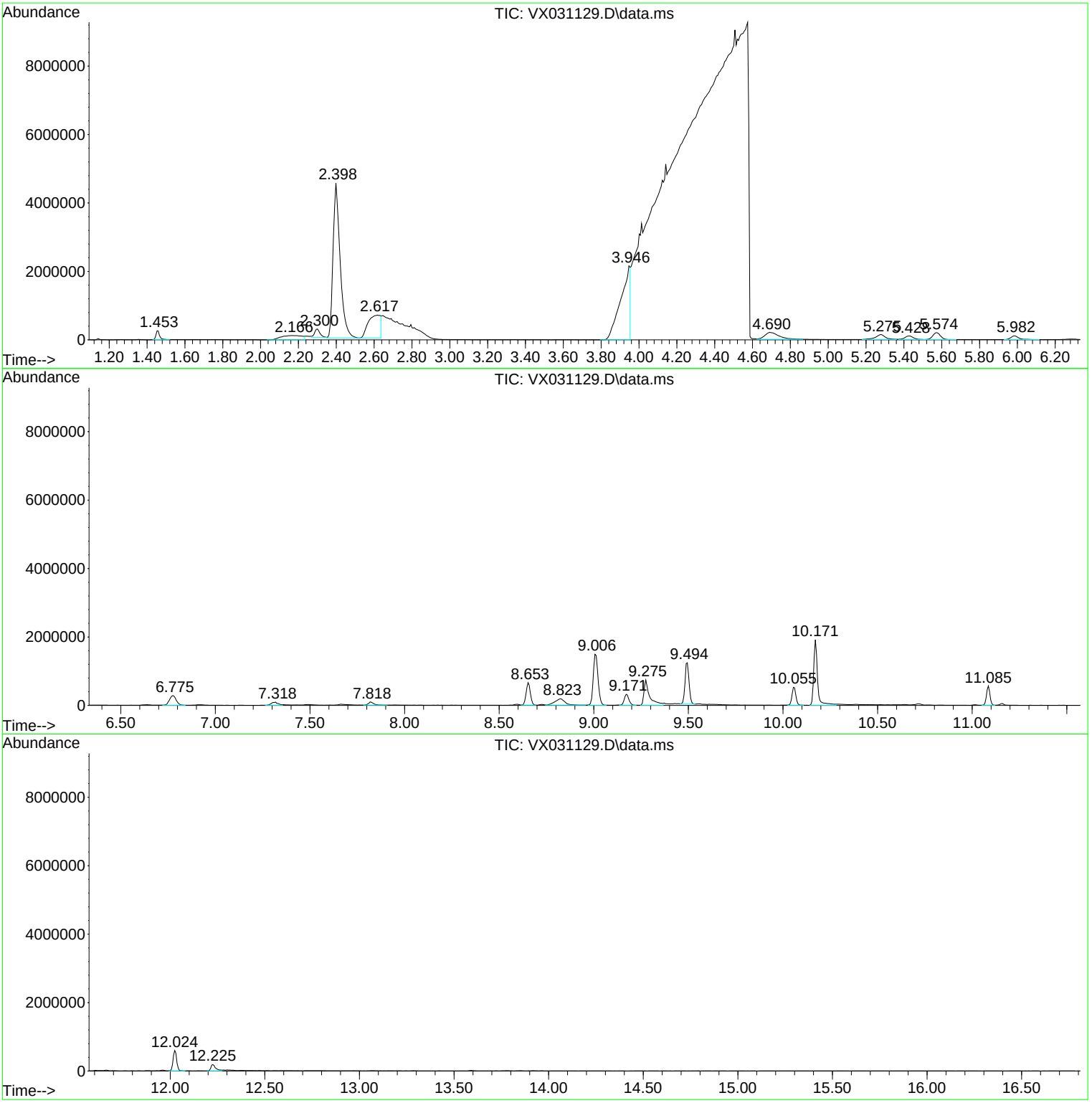
ClientSampleId :
ORA-1504

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

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



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Data File : VX031129.D
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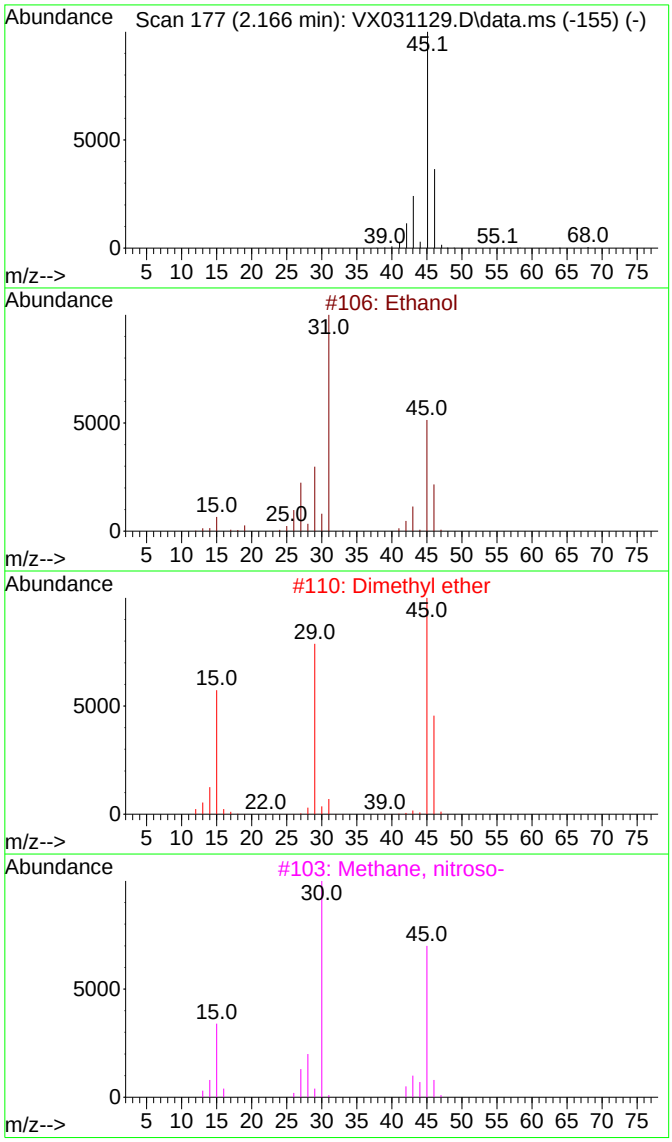
Quant Title : SW846 8260

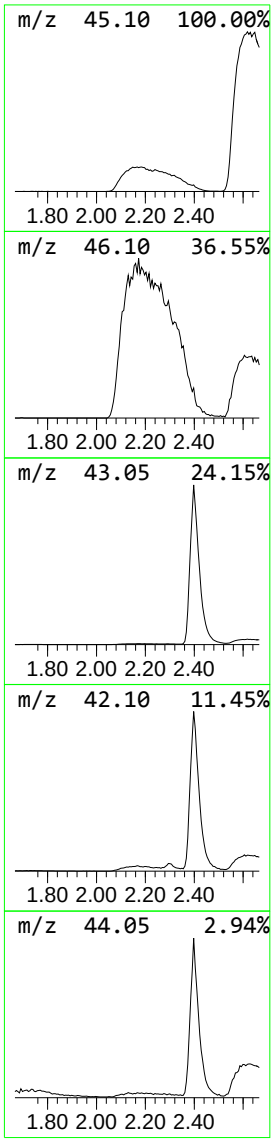
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.166	85.31 ug/l	985648	Pentafluorobenzene	5.574

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	4-Penten-2-ol	86	C5H10O	000625-31-0	2





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Data File : VX031129.D
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1504

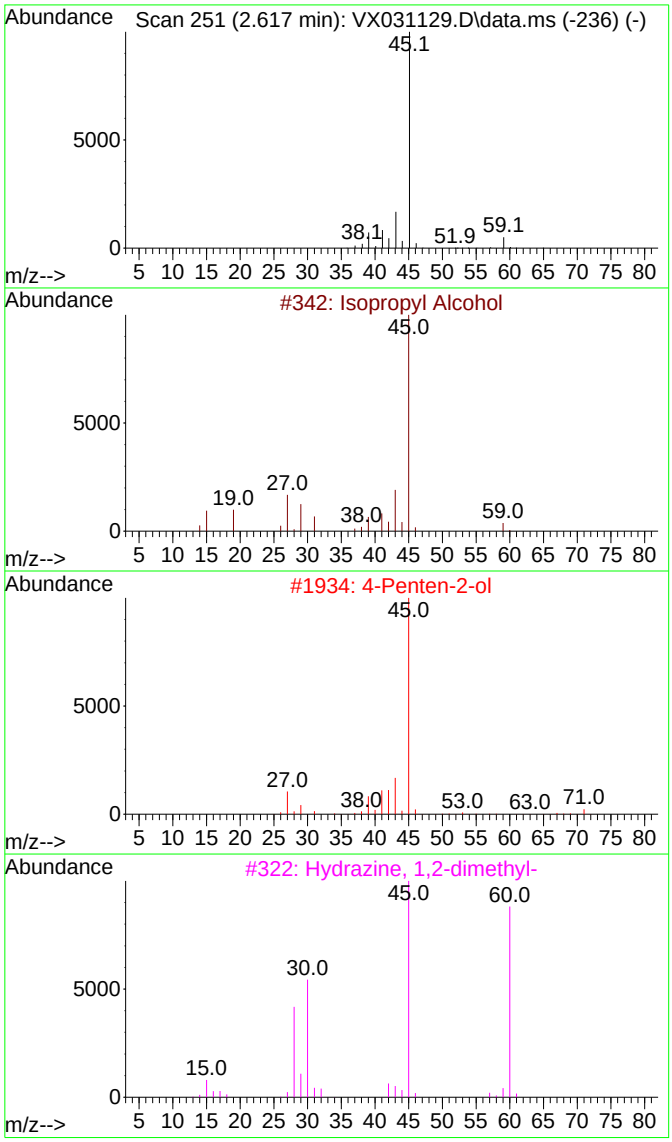
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

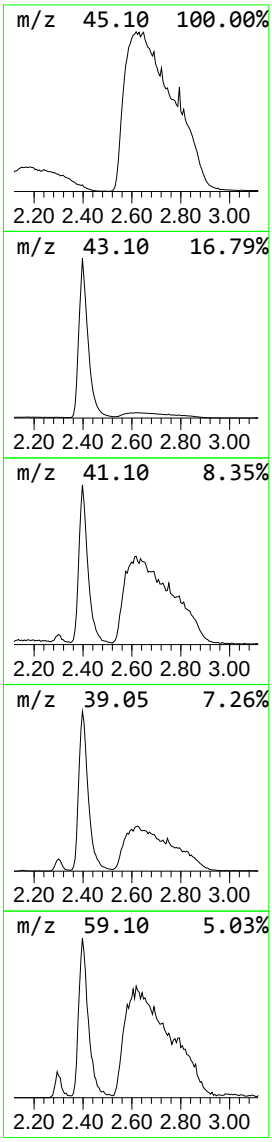
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.617	266.48 ug/l	3078720	Pentafluorobenzene	5.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2	4-Penten-2-ol	86	C5H10O	000625-31-0	9
3	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4	Formamide	45	CH3NO	000075-12-7	7
5	L-Lactic acid	90	C3H6O3	000079-33-4	4





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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1504

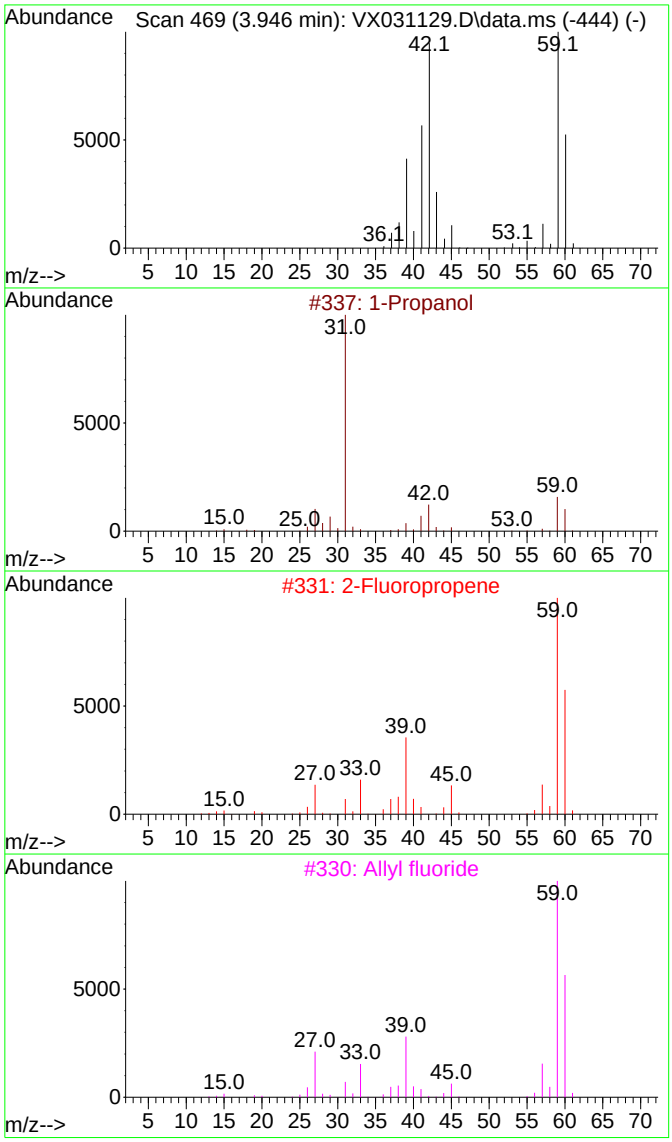
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

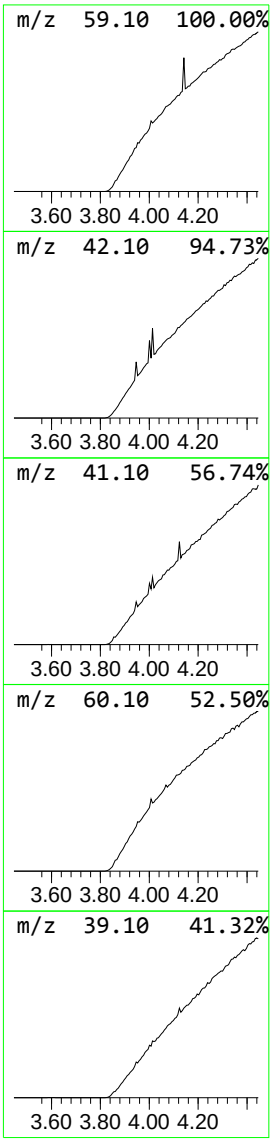
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.946	659.04 ug/l	7614160	Pentafluorobenzene	5.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	64
2	2-Fluoropropene	60	C3H5F	001184-60-7	52
3	Allyl fluoride	60	C3H5F	000818-92-8	38
4	Cyclopropane	42	C3H6	000075-19-4	9
5	Propene	42	C3H6	000115-07-1	9





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Operator : JC/MD
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1504

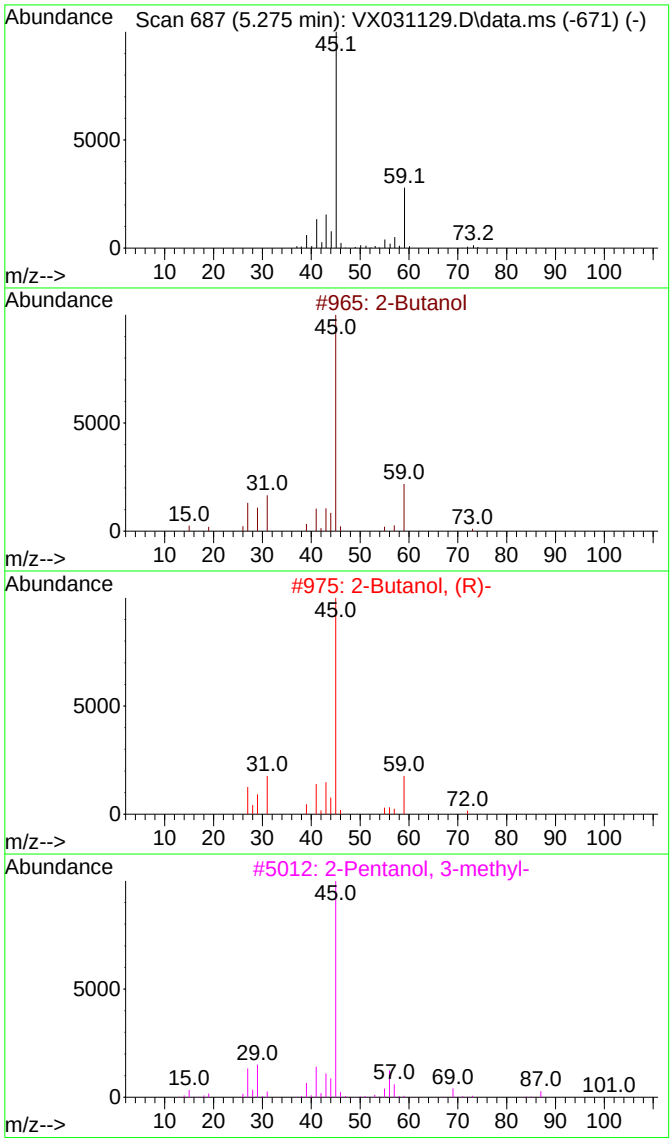
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

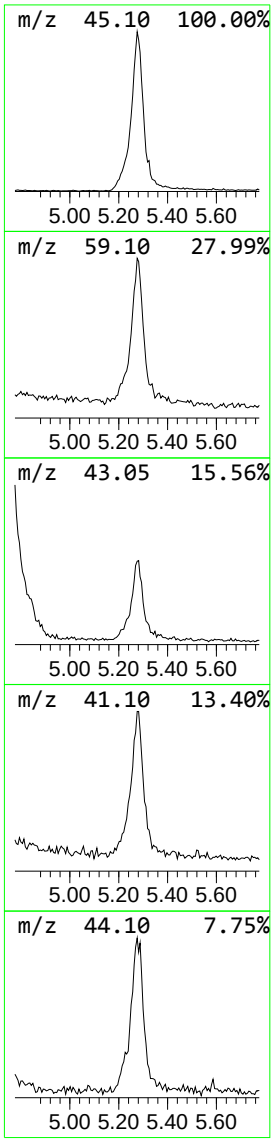
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Butanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.275	44.97 ug/l	519518	Pentafluorobenzene	5.574

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol	74	C4H10O	000078-92-2	83
2	2-Butanol, (R)-	74	C4H10O	014898-79-4	64
3	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	59
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	42
5	2-Hexanol, (R)-	102	C6H14O	026549-24-6	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1504

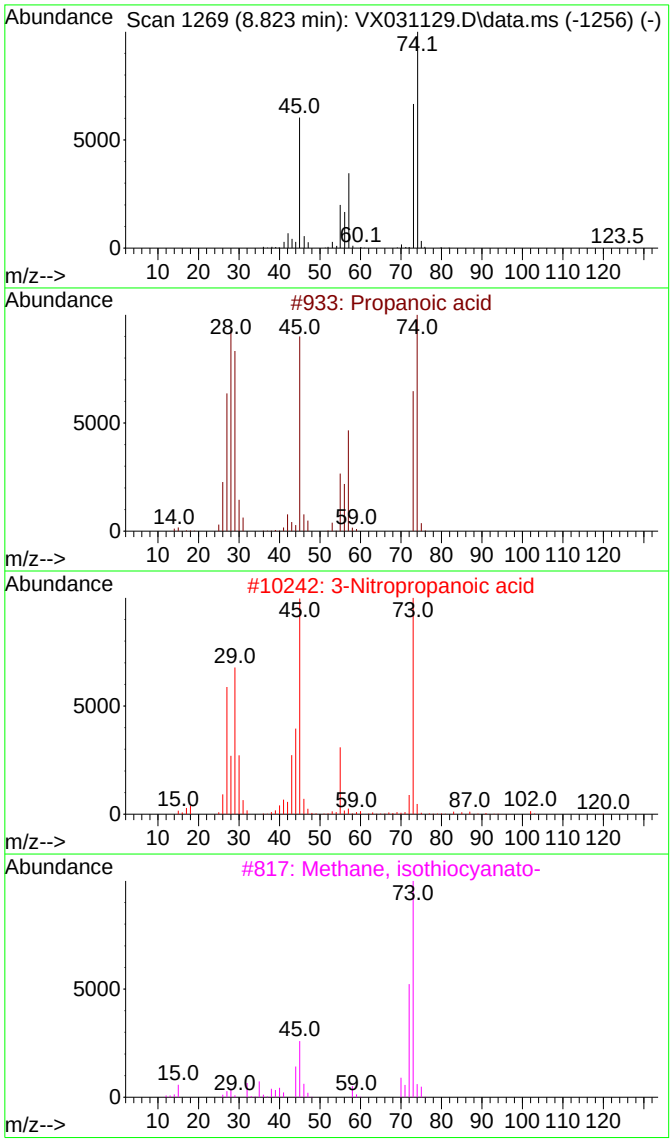
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

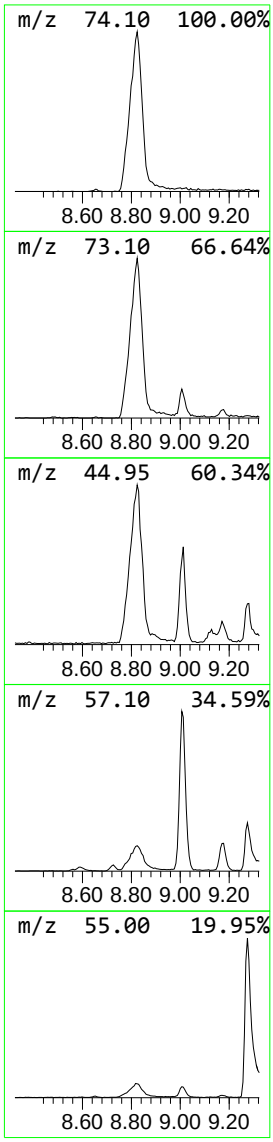
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Propanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.823	45.17 ug/l	674534	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid	74	C3H6O2	000079-09-4	90
2	3-Nitropropanoic acid	119	C3H5NO4	000504-88-1	12
3	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
4	Formic acid, 3-methylbut-2-yl ester	116	C6H12O2	1010367-95-2	9
5	2-Amino-2-methyl-1,3-propanediol	105	C4H11NO2	000115-69-5	9





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1504

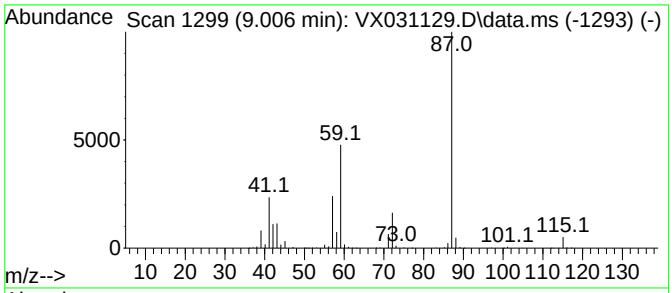
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

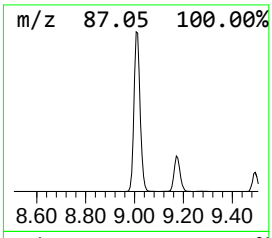
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

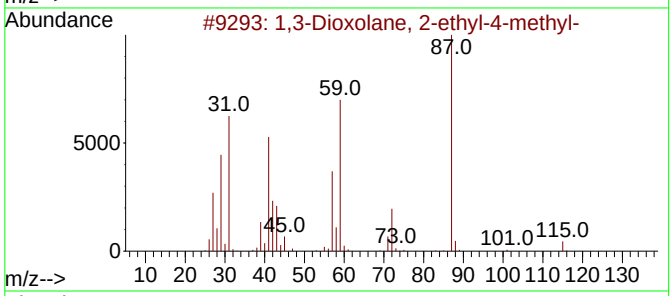
****
Peak Number 7 1,3-Dioxolane, 2-ethyl-4-me... Concentration Rank 4

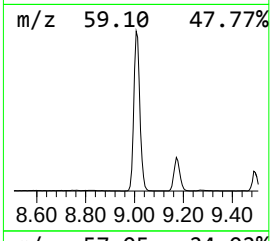
R.T.	EstConc	Area	Relative to ISTD	R.T.
9.006	172.63 ug/l	2577830	Chlorobenzene-d5	10.055

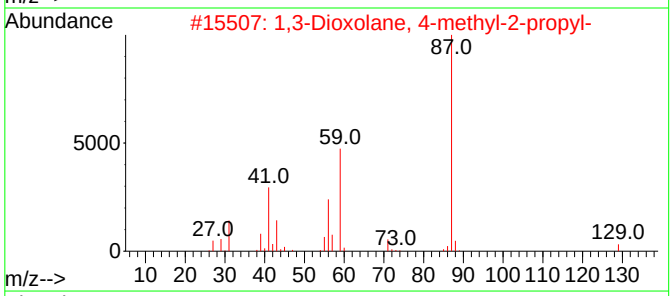
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2-ethyl-4-methyl-	116	C6H12O2	004359-46-0	91
2	1,3-Dioxolane, 4-methyl-2-propyl-	130	C7H14O2	004352-99-2	72
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	53
4	2-Propanone, O-methyloxime	87	C4H9NO	003376-35-0	52
5	Oxazolidin-2-one	87	C3H5NO2	000497-25-6	50

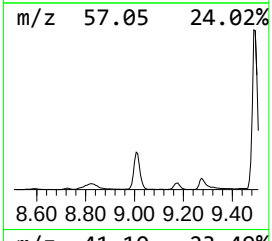


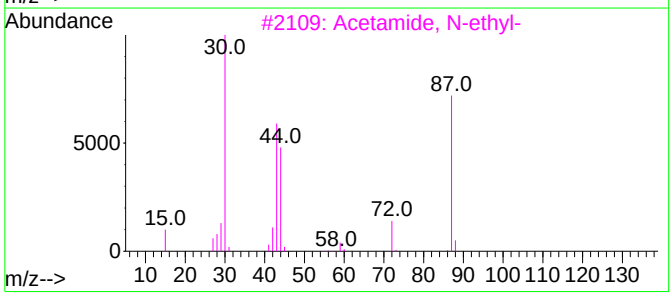


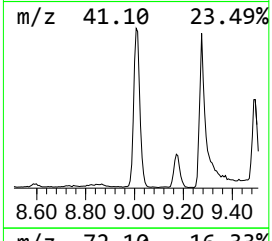


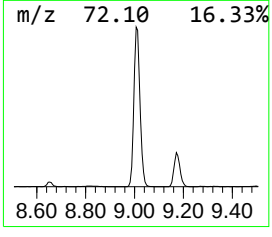












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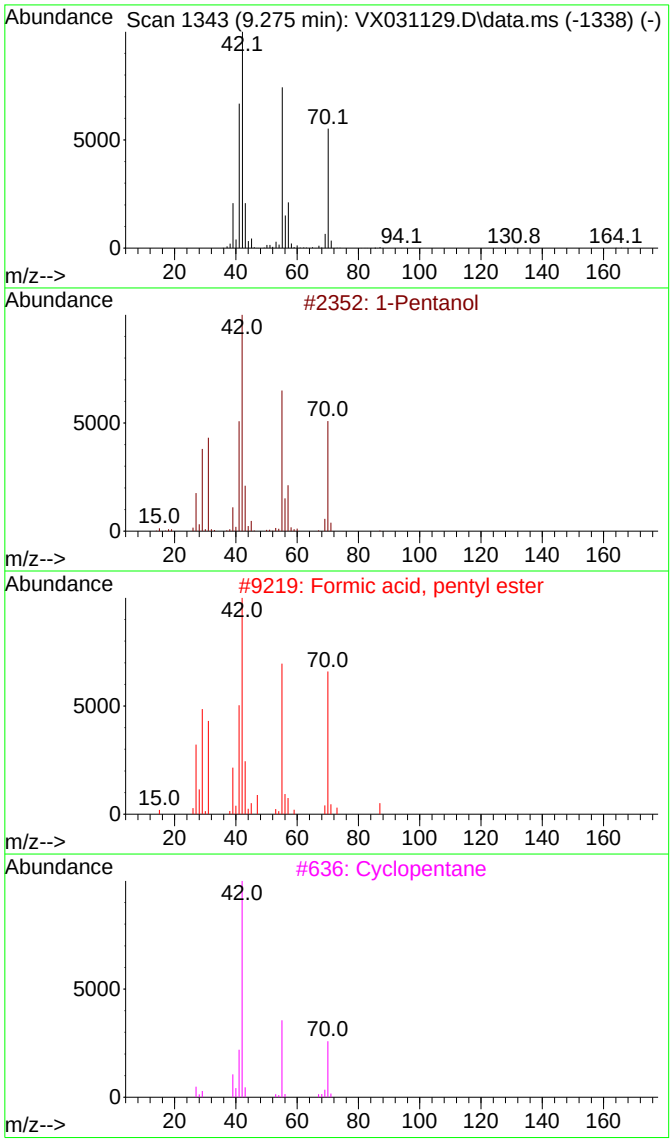
Quant Title : SW846 8260

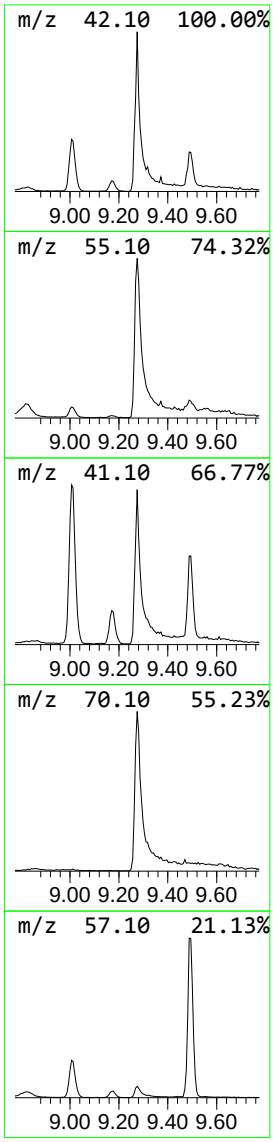
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1-Pentanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.275	101.15 ug/l	1510550	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol	88	C5H12O	000071-41-0	90
2	Formic acid, pentyl ester	116	C6H12O2	000638-49-3	83
3	Cyclopentane	70	C5H10	000287-92-3	72
4	1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	59
5	1-Pentene	70	C5H10	000109-67-1	56





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ClientSampleId :
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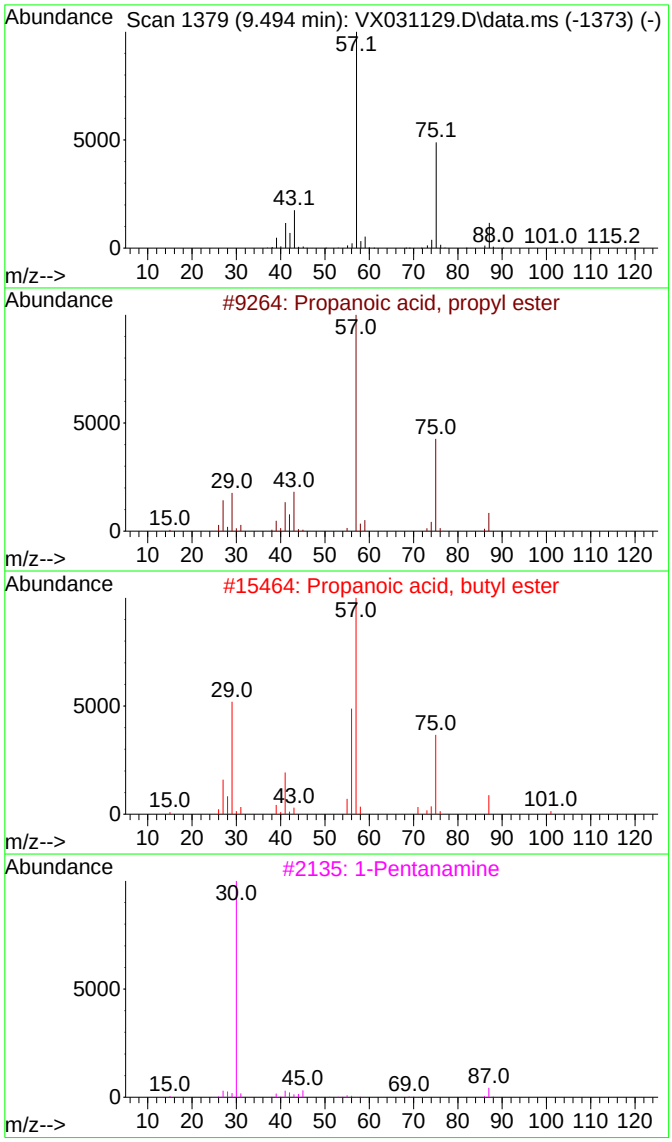
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

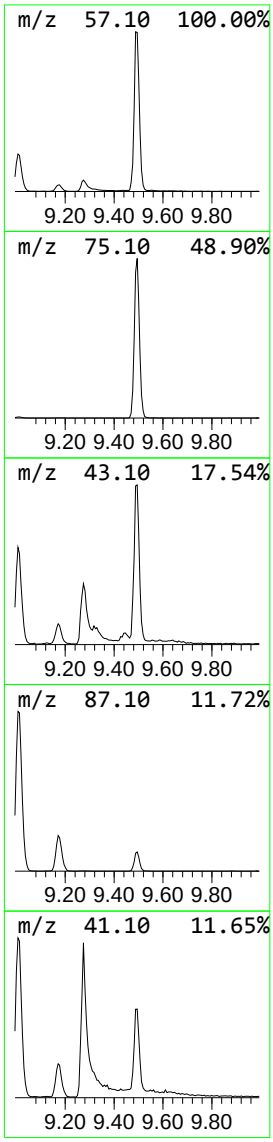
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Propanoic acid, propyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.494	118.92 ug/l	1775870	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	40
3	1-Pentanamine	87	C5H13N	000110-58-7	9
4	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
5	Isobutyl ether	130	C8H18O	000628-55-7	9





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Instrument :
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ClientSampleId :
ORA-1504

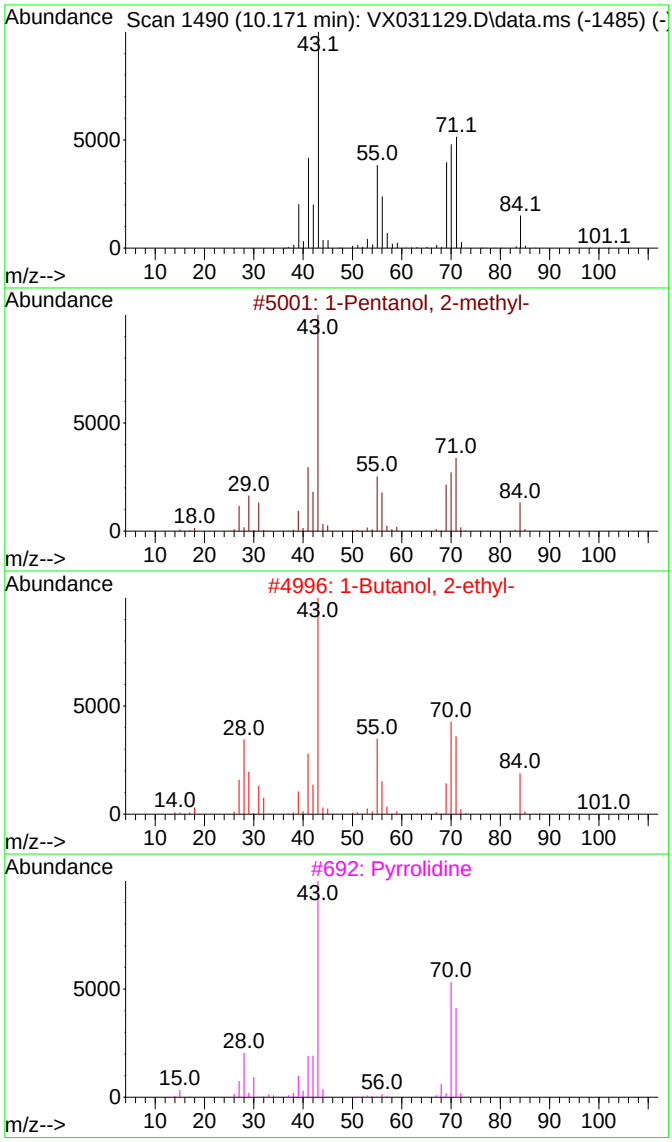
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.M
Quant Title : SW846 8260

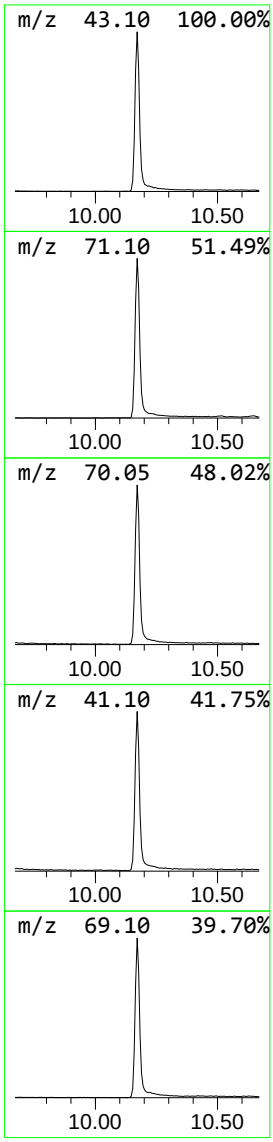
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1-Pentanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.171	181.04 ug/l	2703450	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	90
2	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	90
3	Pyrrolidine	71	C4H9N	000123-75-1	53
4	Formic acid, 2-ethylbutyl ester	130	C7H14O2	1000367-92-2	50
5	1-Trifluoroacetoxy-2-methylpentane	198	C8H13F3O2	155089-96-6	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX090622\
Data File : VX031129.D
Acq On : 06 Sep 2022 15:39
Operator : JC/MD
Sample : N4489-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1504

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X090122W.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
Ethanol	2.166	85.3	ug/l	985648	1	5.574	577669	50.0
Isopropyl Alcohol	2.617	266.5	ug/l	3078720	1	5.574	577669	50.0
1-Propanol	3.946	659.0	ug/l	7614160	1	5.574	577669	50.0
2-Butanol	5.275	45.0	ug/l	519518	1	5.574	577669	50.0
Propanoic acid	8.823	45.2	ug/l	674534	3	10.055	746653	50.0
1,3-Dioxolane, ...	9.006	172.6	ug/l	2577830	3	10.055	746653	50.0
1-Pentanol	9.275	101.2	ug/l	1510550	3	10.055	746653	50.0
Propanoic acid,...	9.494	118.9	ug/l	1775870	3	10.055	746653	50.0
1-Pentanol, 2-m...	10.171	181.0	ug/l	2703450	3	10.055	746653	50.0