LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072723\
Data File : VX036673.D
Acq On : 27 Jul 2023 13:52
Operator : JC/MD
Sample : 03771-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PATERSON-GSMP-COMP

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\82X072123W.M
Title : SW846 8260

Signal : TIC: VX036673.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	25	28	37	rBV	110570	121135	1.16%	0.317%
2	2.386	206	213	230	rBV	5647190	10480119	100.00%	27.461%
3	2.556	233	241	262	rVB	3317079	6308618	60.20%	16.530%
4	3.861	442	455	472	rBV	196115	499558	4.77%	1.309%
5	4.562	558	570	592	rBV	1734474	4860132	46.37%	12.735%
6	5.013	631	644	664	rBV	583187	1868913	17.83%	4.897%
7	5.385	696	705	722	rVB	89999	267663	2.55%	0.701%
8	5.550	722	732	752	rVB	149833	427866	4.08%	1.121%
9	5.958	786	799	810	rBV	97428	260878	2.49%	0.684%
10	6.641	900	911	922	rBV	40904	107550	1.03%	0.282%
11	6.763	922	931	948	rVB	246177	581721	5.55%	1.524%
12	7.214	998	1005	1013	rBV	213288	449779	4.29%	1.179%
13	7.458	1036	1045	1060	rVB	3242153	6361282	60.70%	16.668%
14	7.641	1069	1075	1082	rVB	108467	185829	1.77%	0.487%
15	7.903	1110	1118	1141	rBV	849755	1541517	14.71%	4.039%
16	8.647	1234	1240	1247	rBV	503785	797726	7.61%	2.090%
17	8.720	1247	1252	1257	rBV	213772	326932	3.12%	0.857%
18	9.238	1331	1337	1345	rBV	183753	298284	2.85%	0.782%
19	9.433	1364	1369	1374	rBV	111057	146802	1.40%	0.385%
20	10.055	1459	1471	1482	rBV	536972	737837	7.04%	1.933%
21	10.153	1482	1487	1494	rBV	108743	151668	1.45%	0.397%
22	10.579	1552	1557	1564	rBV	109722	148630	1.42%	0.389%
23	11.079	1632	1639	1650	rBV	428407	557804	5.32%	1.462%
24	12.024	1788	1794	1801	rBV	510932	675849	6.45%	1.771%

Sum of corrected areas: 38164092

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Instrument :
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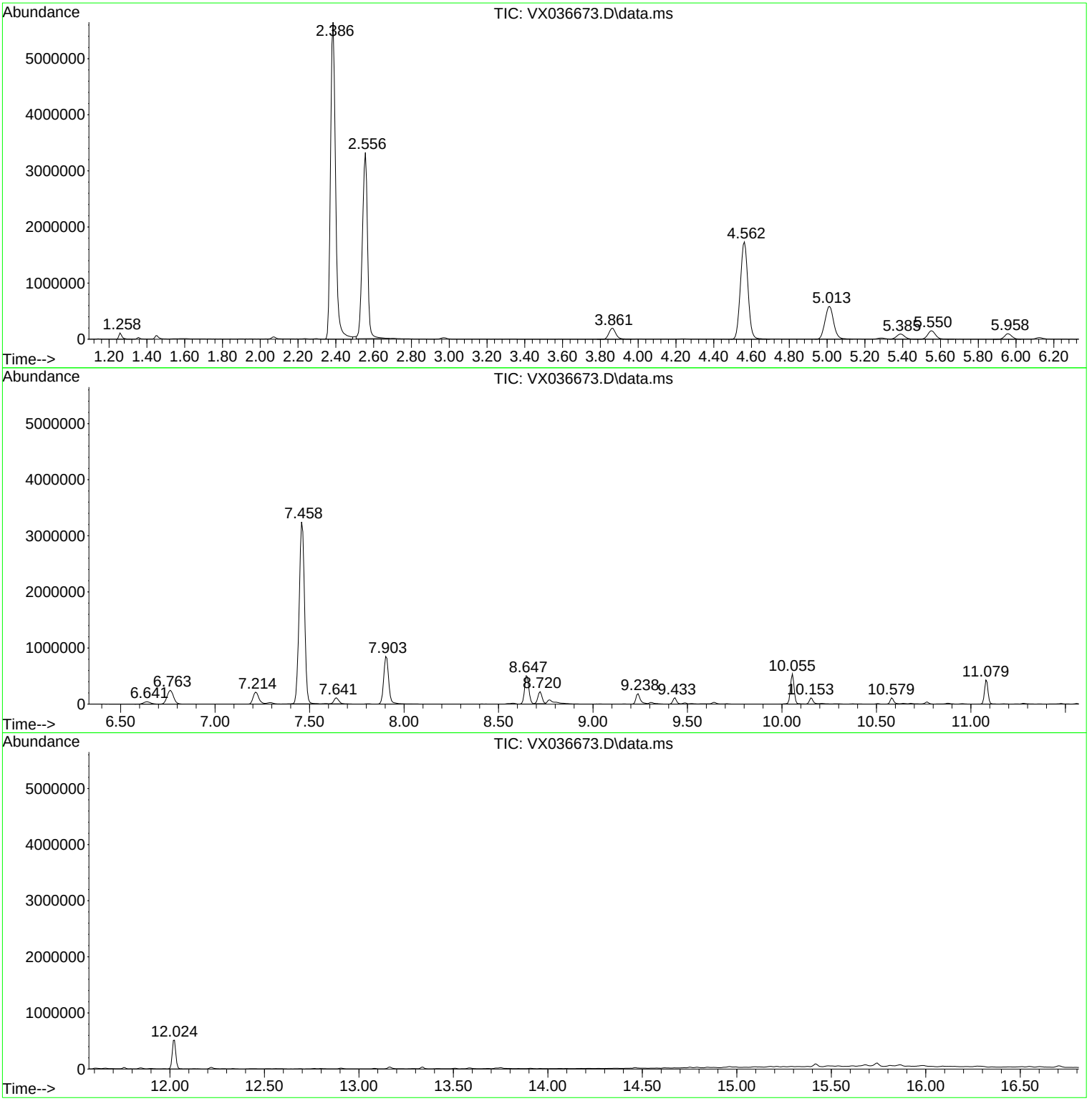
ClientSampleId :
PATERSON-GSMP-COMP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
PATERSON-GSMP-COMP

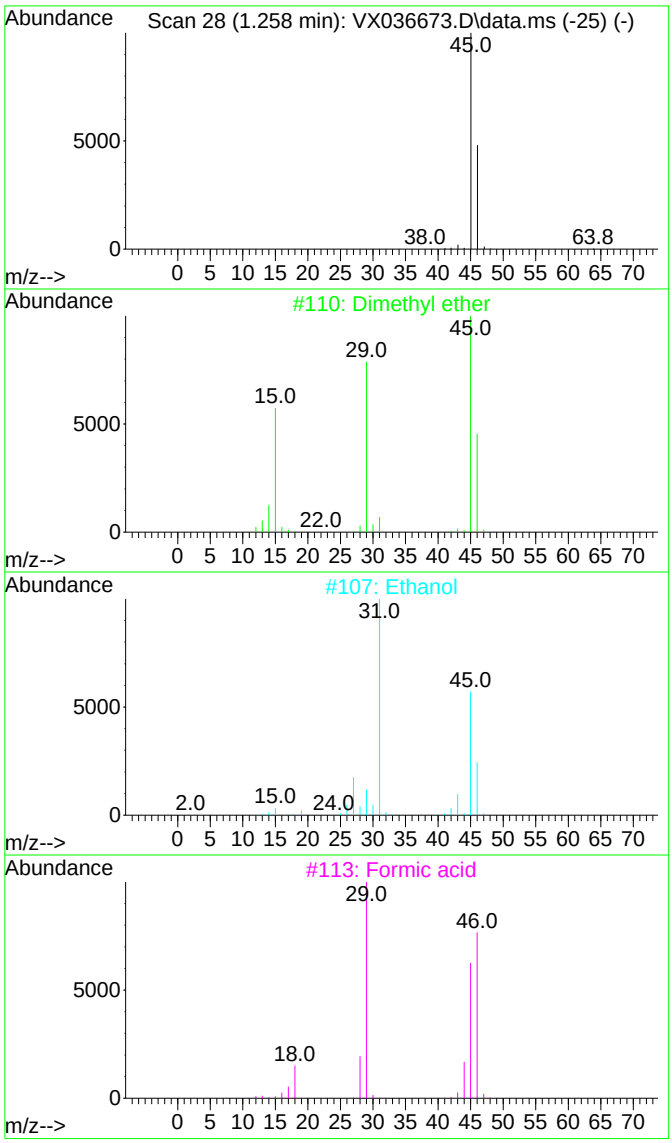
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

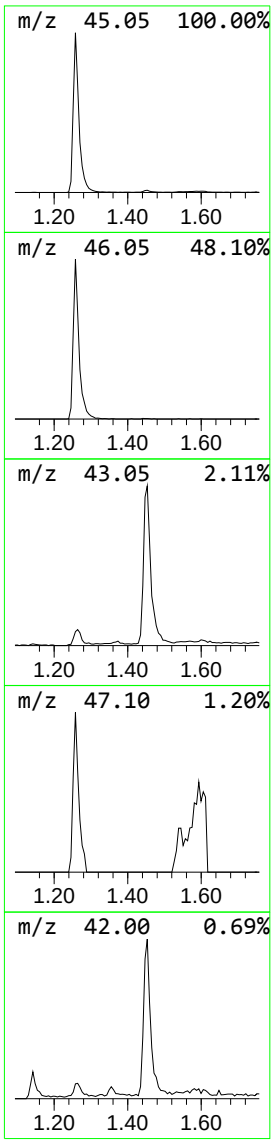
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Dimethyl ether Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	14.16 ug/l	121135	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	5
4	Oxalic acid	90	C2H2O4	000144-62-7	4
5	Methane, nitroso-	45	CH3NO	000865-40-7	3





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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PATERSON-GSMP-COMP

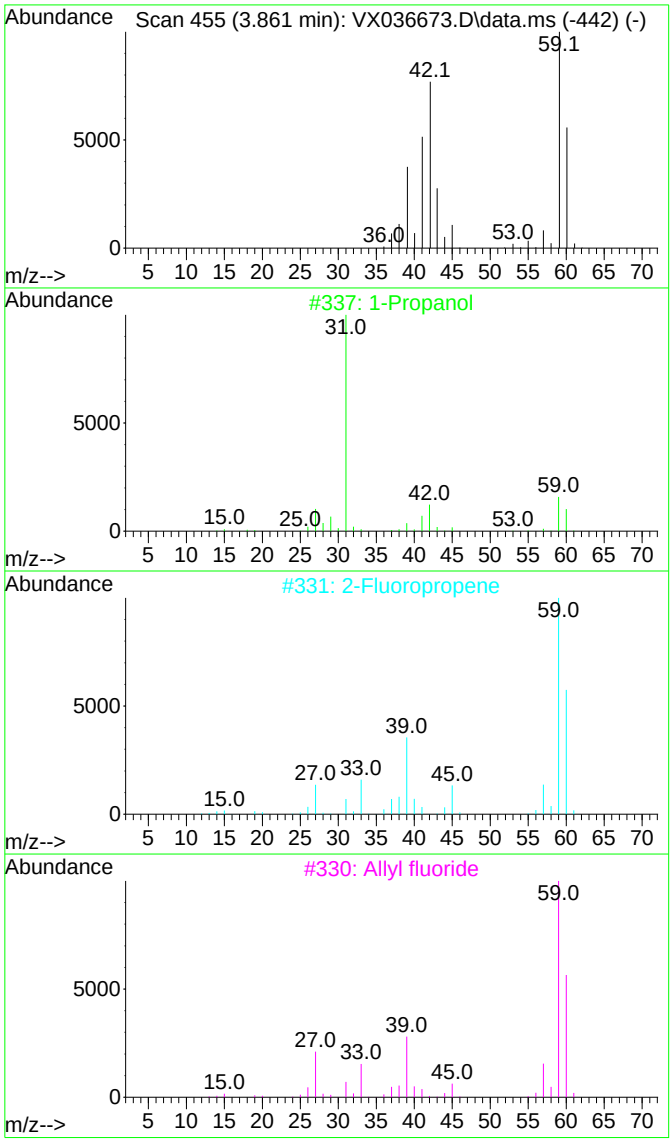
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

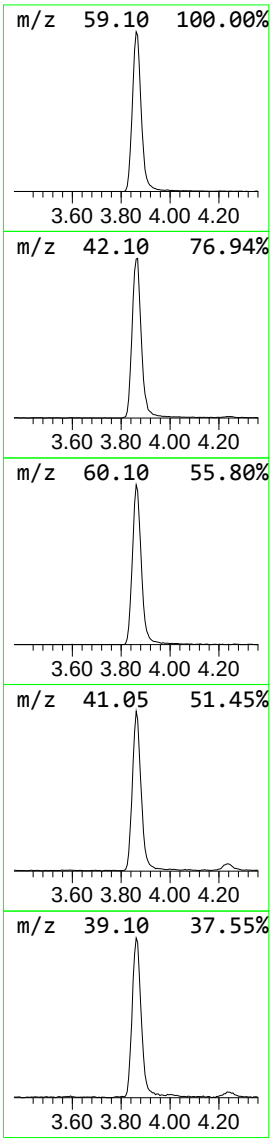
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Propanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.861	58.38 ug/l	499558	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	78
2	2-Fluoropropene	60	C3H5F	001184-60-7	43
3	Allyl fluoride	60	C3H5F	000818-92-8	38
4	Cyclopropane	42	C3H6	000075-19-4	27
5	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	7





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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PATERSON-GSMP-COMP

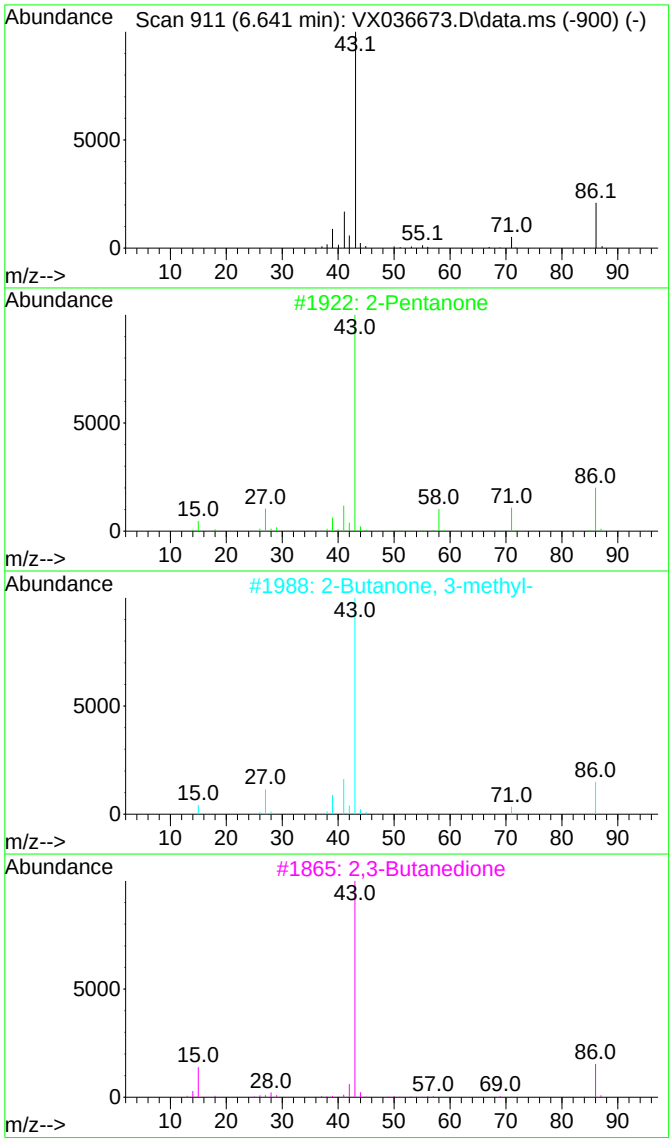
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

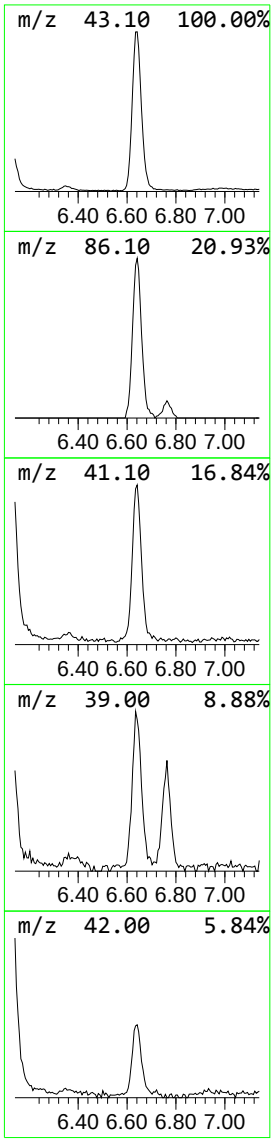
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.641	9.24 ug/l	107550	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	72
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	72
3	2,3-Butanedione	86	C4H6O2	000431-03-8	64
4	3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	38
5	2,3-Hexanedione	114	C6H10O2	003848-24-6	9





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PATERSON-GSMP-COMP

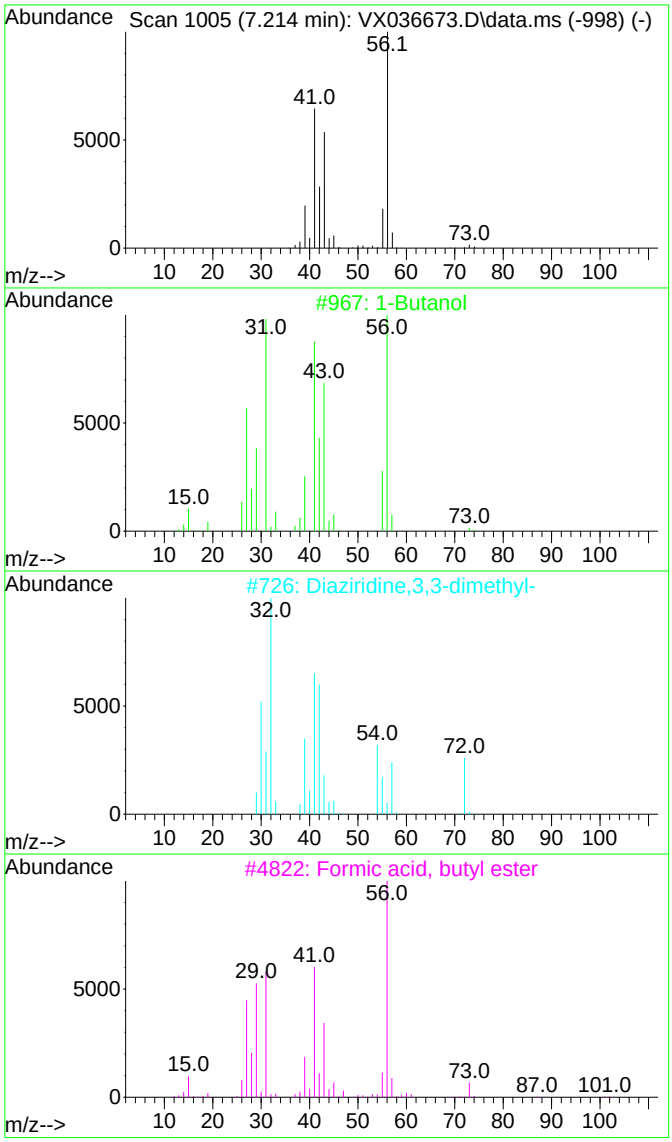
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

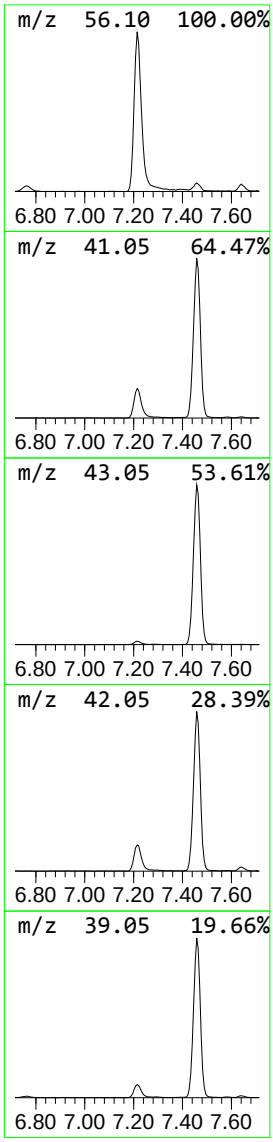
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.214	38.66 ug/l	449779	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	90
2	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9
3	Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
4	3-Butenoic acid, 2-amino-	101	C4H7NO2	056512-51-7	9
5	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	9





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Acq On : 27 Jul 2023 13:52
Operator : JC/MD
Sample : 03771-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PATERSON-GSMP-COMP

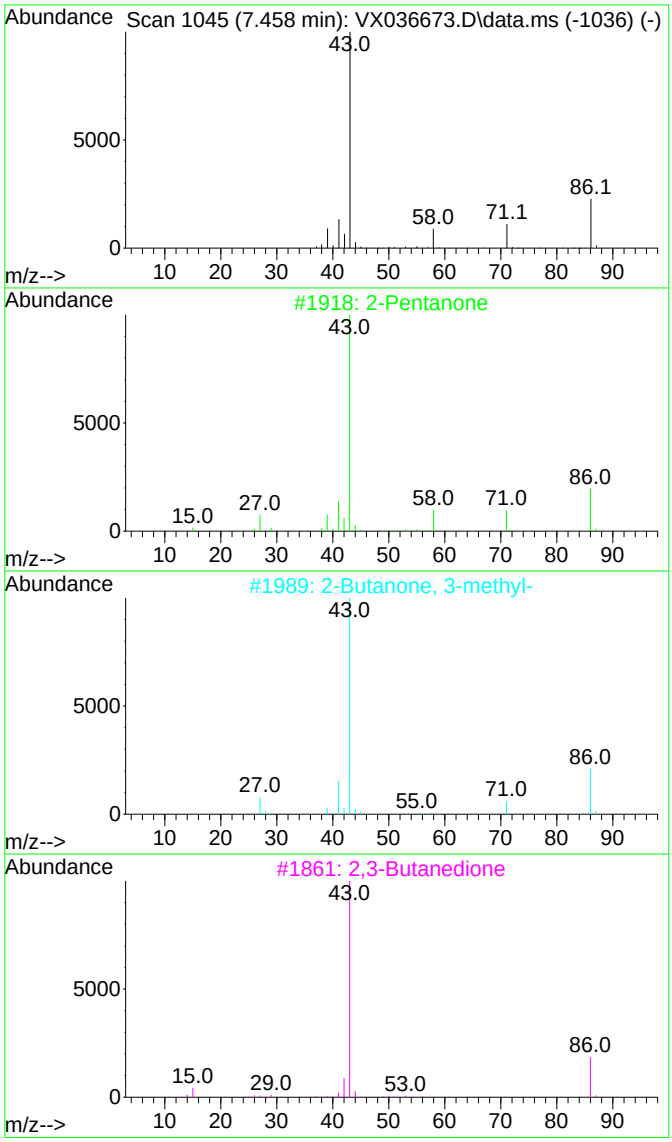
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

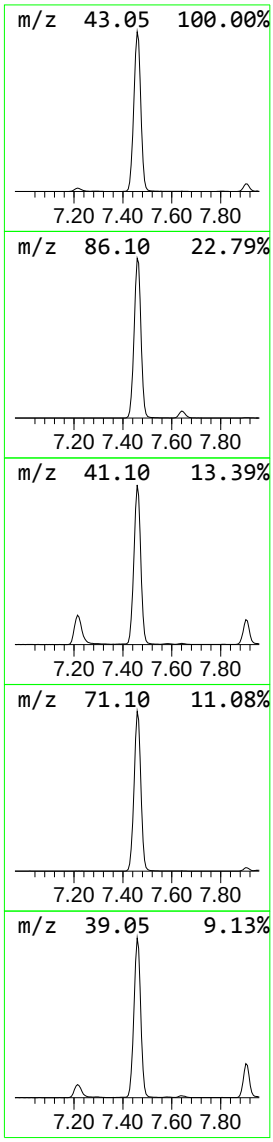
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2-Butanone, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.458	546.76 ug/l	6361280	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	52
4	3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	36
5	Butane	58	C4H10	000106-97-8	9





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PATERSON-GSMP-COMP

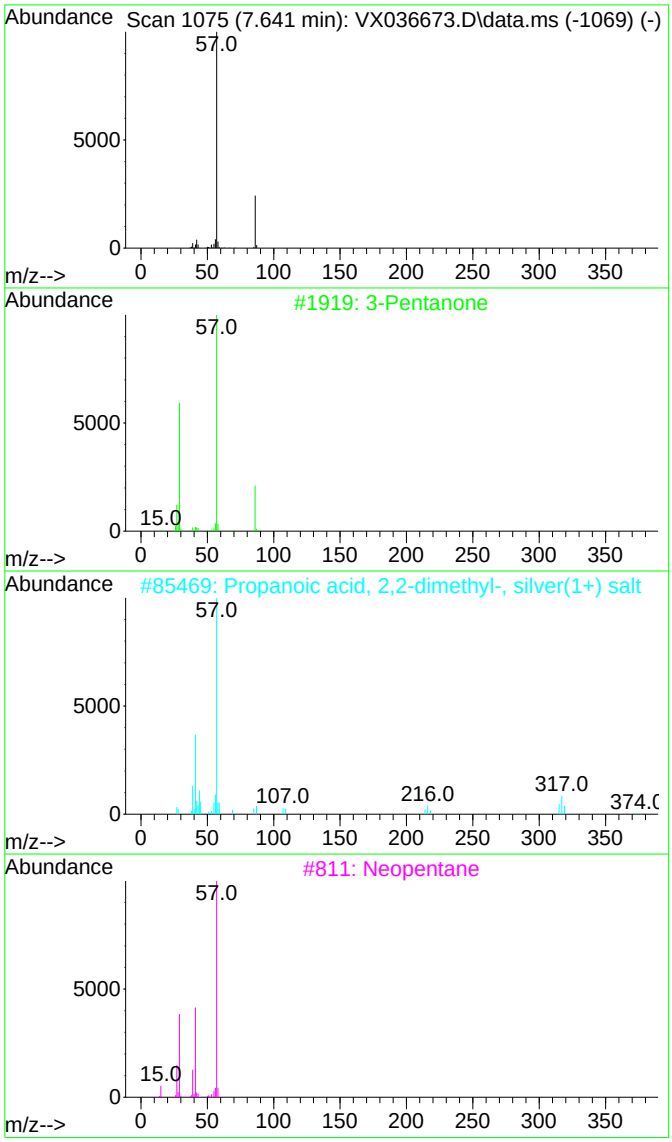
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

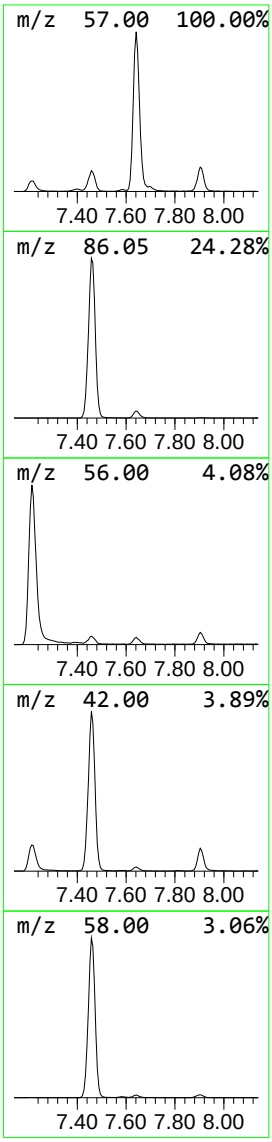
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 3-Pentanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.641	15.97 ug/l	185829	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	80
2	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	9
3	Neopentane	72	C5H12	000463-82-1	9
4	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	7
5	Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	7





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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PATERSON-GSMP-COMP

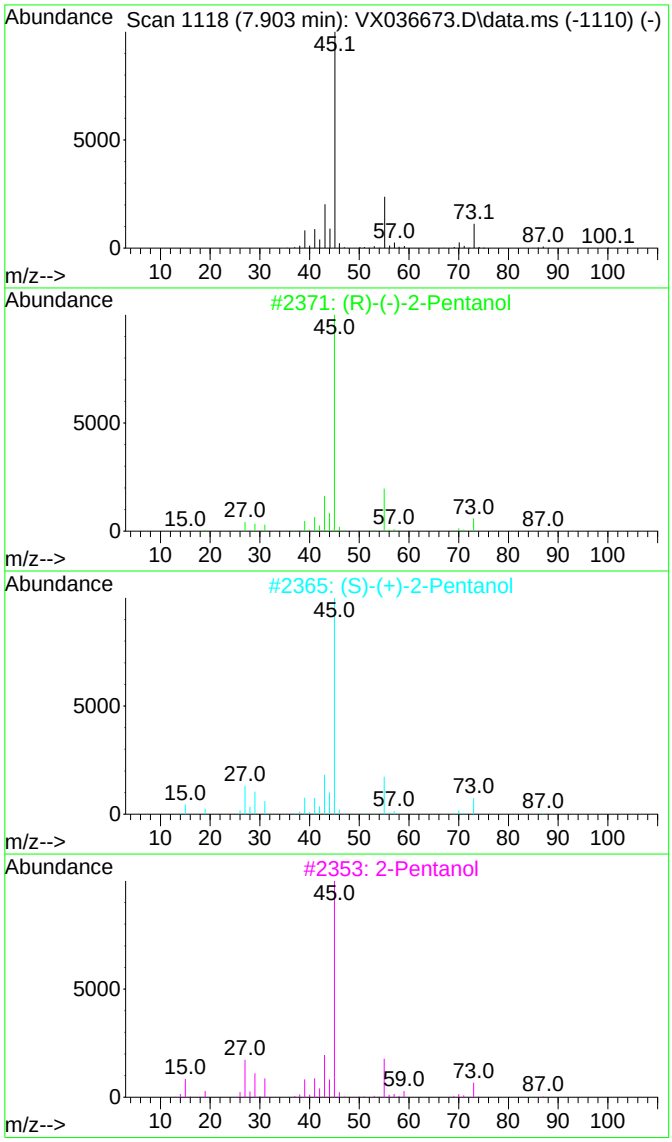
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

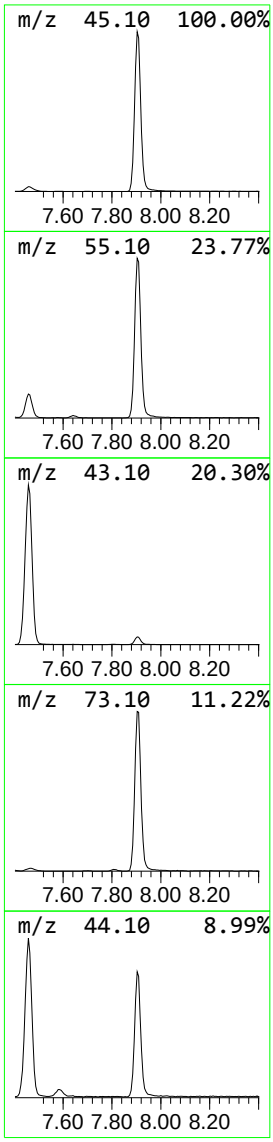
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 (R)-(-)-2-Pentanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.903	132.50 ug/l	1541520	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	83
2	(S)-(+)-2-Pentanol	88	C5H12O	026184-62-3	78
3	2-Pentanol	88	C5H12O	006032-29-7	78
4	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	64
5	2-Butanol, 3-methyl-, (S)-	88	C5H12O	001517-66-4	56





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MSVOA_X
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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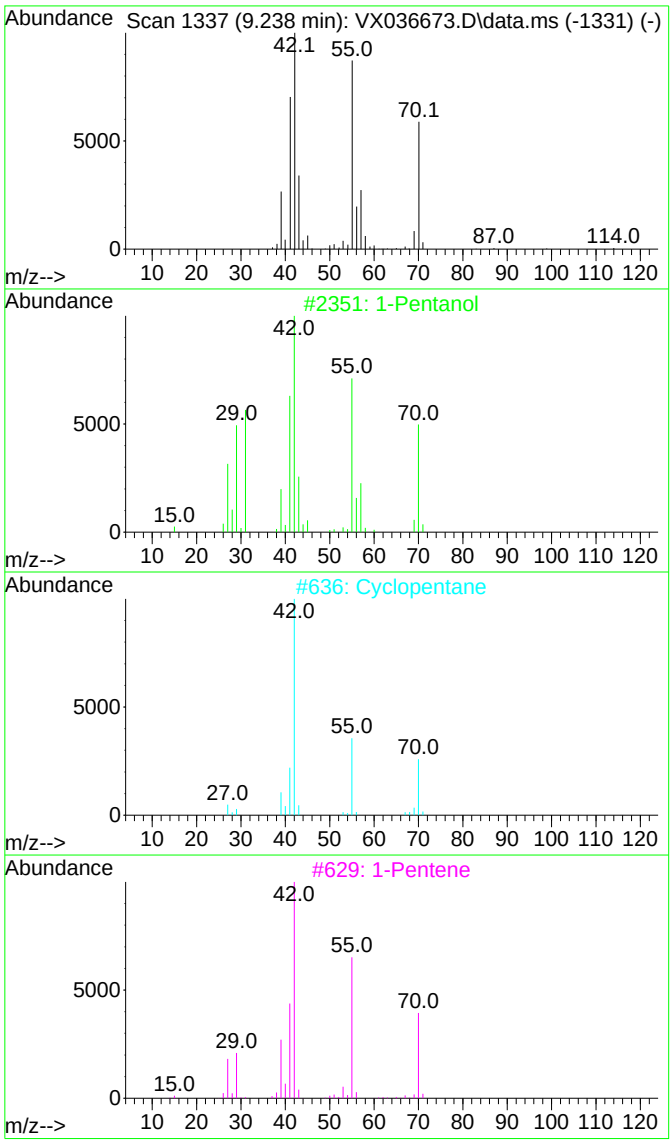
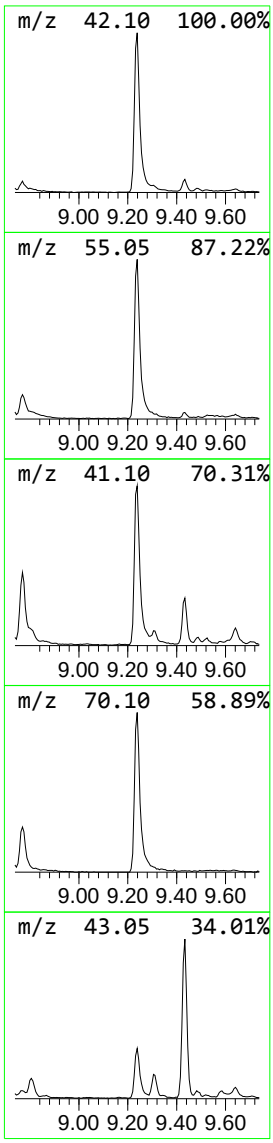
****
Peak Number 8 1-Pentanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.238	20.21 ug/l	298284	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol	88	C5H12O	000071-41-0	90
2	Cyclopentane	70	C5H10	000287-92-3	64
3	1-Pentene	70	C5H10	000109-67-1	64
4	Pentane, 1-chloro-	106	C5H11Cl	000543-59-9	50
5	2(3H)-Furanone, dihydro-3,5-dime...	114	C6H10O2	005145-01-7	39





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MSVOA_X
ClientSampleId :
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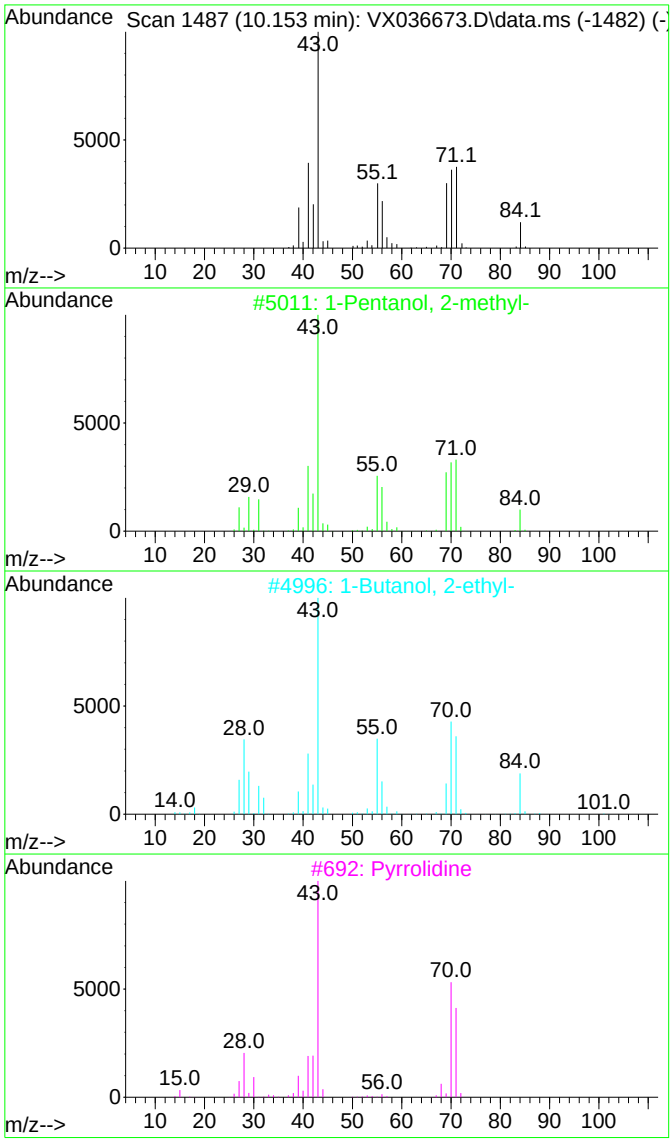
Quant Title : SW846 8260

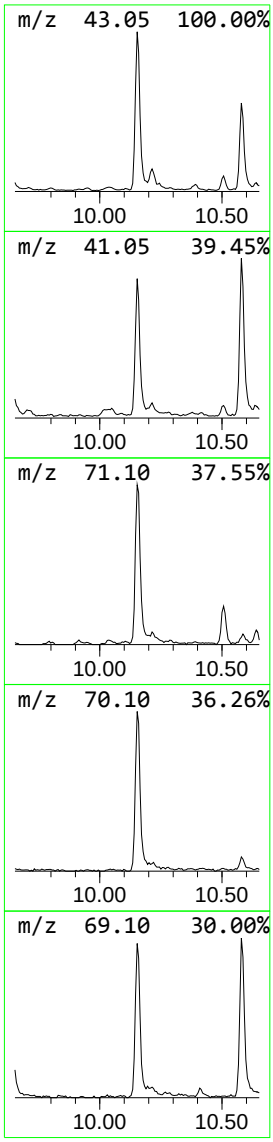
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1-Pentanol, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.153	10.28 ug/l	151668	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	72
3	Pyrrolidine	71	C4H9N	000123-75-1	47
4	Butane, 1-bromo-3-methyl-	150	C5H11Br	000107-82-4	38
5	Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	38





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Instrument :
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ClientSampleId :
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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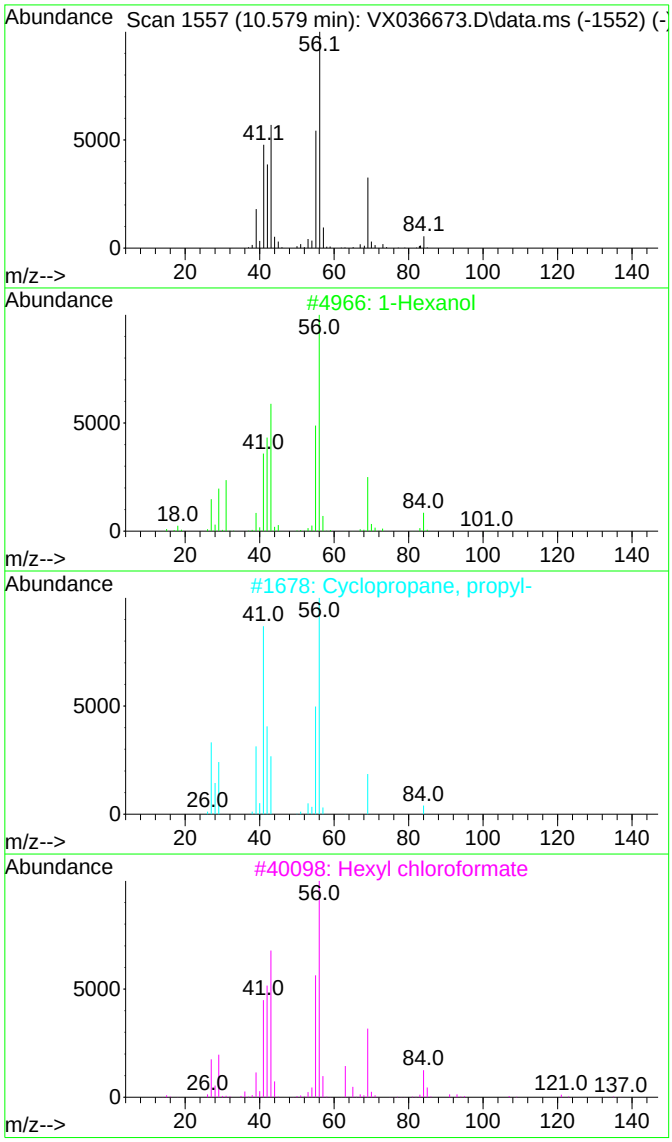
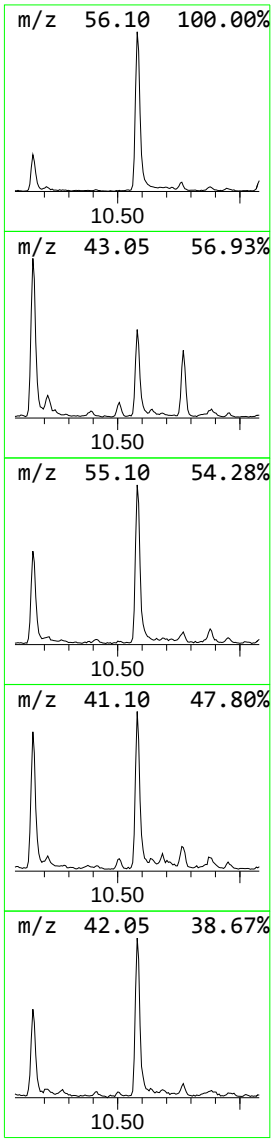
****
Peak Number 10 1-Hexanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.579	10.07 ug/l	148630	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol	102	C6H14O	000111-27-3	83
2	Cyclopropane, propyl-	84	C6H12	002415-72-7	83
3	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	78
4	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	78
5	Cyclobutane, butyl-	112	C8H16	013152-44-8	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072723\
Data File : VX036673.D
Acq On : 27 Jul 2023 13:52
Operator : JC/MD
Sample : 03771-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
PATERSON-GSMP-COMP

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.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	1.258	14.2	ug/l	121135	1	5.550	427866	50.0
1-Propanol	3.861	58.4	ug/l	499558	1	5.550	427866	50.0
2-Pentanone	6.641	9.2	ug/l	107550	2	6.763	581721	50.0
1-Butanol	7.214	38.7	ug/l	449779	2	6.763	581721	50.0
2-Butanone, 3-m...	7.458	546.8	ug/l	6361280	2	6.763	581721	50.0
3-Pentanone	7.641	16.0	ug/l	185829	2	6.763	581721	50.0
(R)-(-)-2-Pentanol	7.903	132.5	ug/l	1541520	2	6.763	581721	50.0
1-Pentanol	9.238	20.2	ug/l	298284	3	10.055	737837	50.0
1-Pentanol, 2-m...	10.153	10.3	ug/l	151668	3	10.055	737837	50.0
1-Hexanol	10.579	10.1	ug/l	148630	3	10.055	737837	50.0