LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039599.D
Acq On : 03 Jan 2024 14:05
Operator : JC/MD
Sample : P1002-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1211

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: VX039599.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	20	rBV2	165669	181753	1.26%	0.517%
2	1.252	24	27	41	rBV	11676012	14386488	100.00%	40.892%
3	1.356	41	44	53	rVB2	126191	158330	1.10%	0.450%
4	2.099	156	166	179	rBV	130118	311534	2.17%	0.886%
5	2.380	205	212	228	rBV	694919	1211618	8.42%	3.444%
6	2.959	298	307	326	rBV2	103831	321369	2.23%	0.913%
7	3.690	415	427	447	rBV	376330	1013550	7.05%	2.881%
8	4.221	500	514	523	rBV3	214145	668169	4.64%	1.899%
9	4.312	524	529	552	rVB5	40033	194558	1.35%	0.553%
10	4.556	560	569	588	rVB	182202	535448	3.72%	1.522%
11	5.385	695	705	718	rBV2	66682	194343	1.35%	0.552%
12	5.544	722	731	749	rVB	95091	276824	1.92%	0.787%
13	5.952	788	798	806	rBV2	77768	205854	1.43%	0.585%
14	6.141	822	829	846	rVB2	65020	198936	1.38%	0.565%
15	6.757	921	930	946	rVB2	180975	442021	3.07%	1.256%
16	7.226	1000	1007	1026	rBV	287315	694235	4.83%	1.973%
17	7.458	1035	1045	1052	rBV	107308	231349	1.61%	0.658%
18	8.647	1234	1240	1246	rBV	390284	611351	4.25%	1.738%
19	8.714	1246	1251	1257	rVV	108757	177329	1.23%	0.504%
20	8.775	1257	1261	1270	rVB2	103797	185286	1.29%	0.527%
21	10.049	1462	1470	1476	rBV	428720	653764	4.54%	1.858%
22	10.153	1483	1487	1491	rBV	157751	223526	1.55%	0.635%
23	10.299	1506	1511	1520	rVB	180429	260116	1.81%	0.739%
24	10.506	1540	1545	1551	rVB	150466	194911	1.35%	0.554%
25	10.640	1562	1567	1570	rBV	113594	149270	1.04%	0.424%
26	10.683	1570	1574	1581	rVB	494083	607438	4.22%	1.727%
27	10.756	1581	1586	1593	rBV3	279891	438918	3.05%	1.248%
28	11.079	1633	1639	1644	rBV	376914	506423	3.52%	1.439%
29	11.128	1644	1647	1652	rVB	265400	329785	2.29%	0.937%
30	11.573	1713	1720	1722	rBV2	197597	320148	2.23%	0.910%
31	11.604	1722	1725	1734	rVV3	164562	283494	1.97%	0.806%
32	11.683	1734	1738	1744	rVB	280738	338899	2.36%	0.963%
33	11.866	1765	1768	1779	rVB3	98931	240847	1.67%	0.685%
34	12.018	1789	1793	1797	rBV	430912	581872	4.04%	1.654%
35	12.219	1821	1826	1836	rBV	6193743	7492780	52.08%	21.297%
36	12.305	1836	1840	1854	rVB	198382	359002	2.50%	1.020%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039599.D
Acq On : 03 Jan 2024 14:05
Operator : JC/MD
Sample : P1002-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1211

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

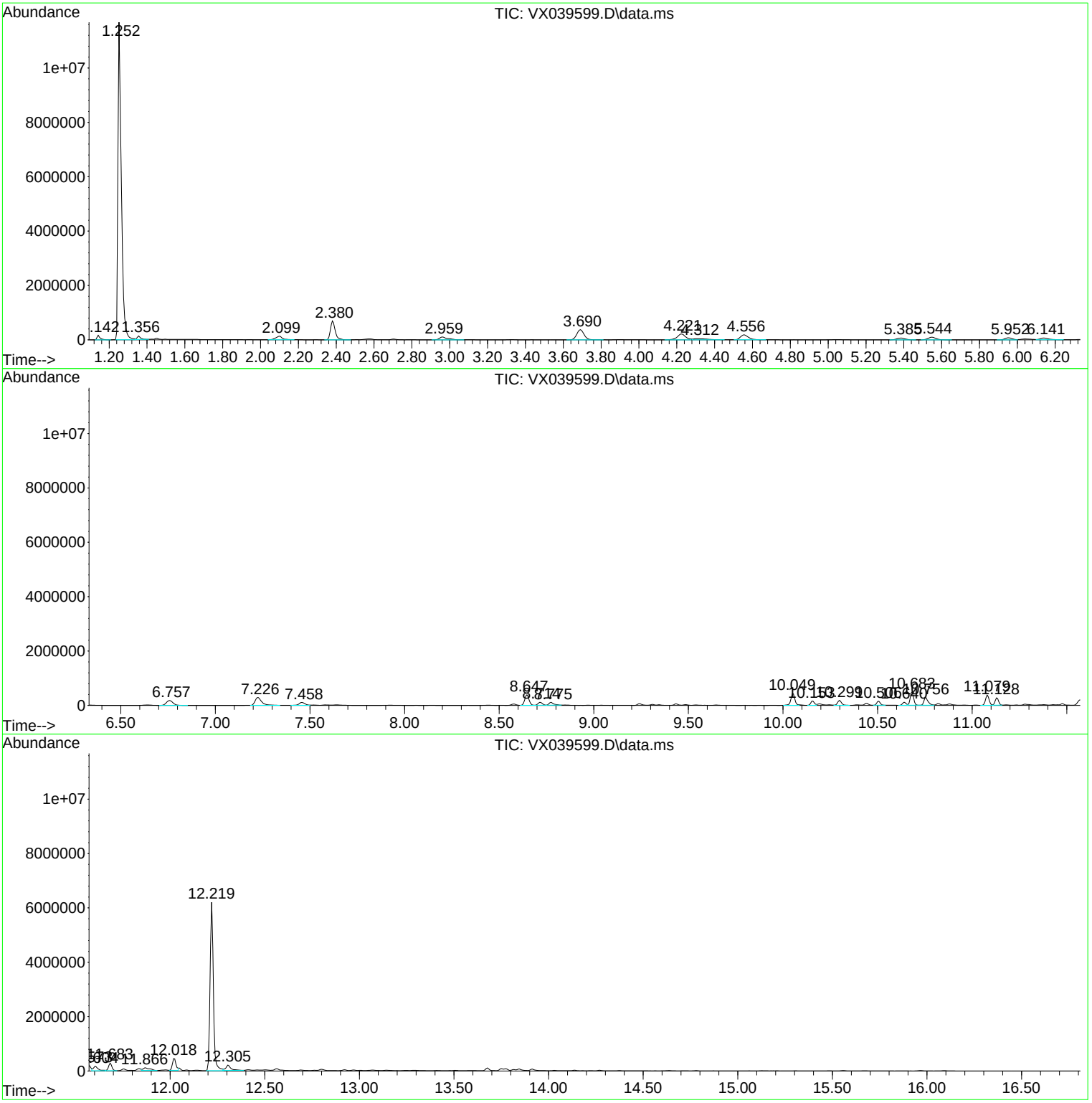
Sum of corrected areas: 35181538

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039599.D
Acq On : 03 Jan 2024 14:05
Operator : JC/MD
Sample : P1002-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1211

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 : VX039599.D
Acq On : 03 Jan 2024 14:05
Operator : JC/MD
Sample : P1002-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1211

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

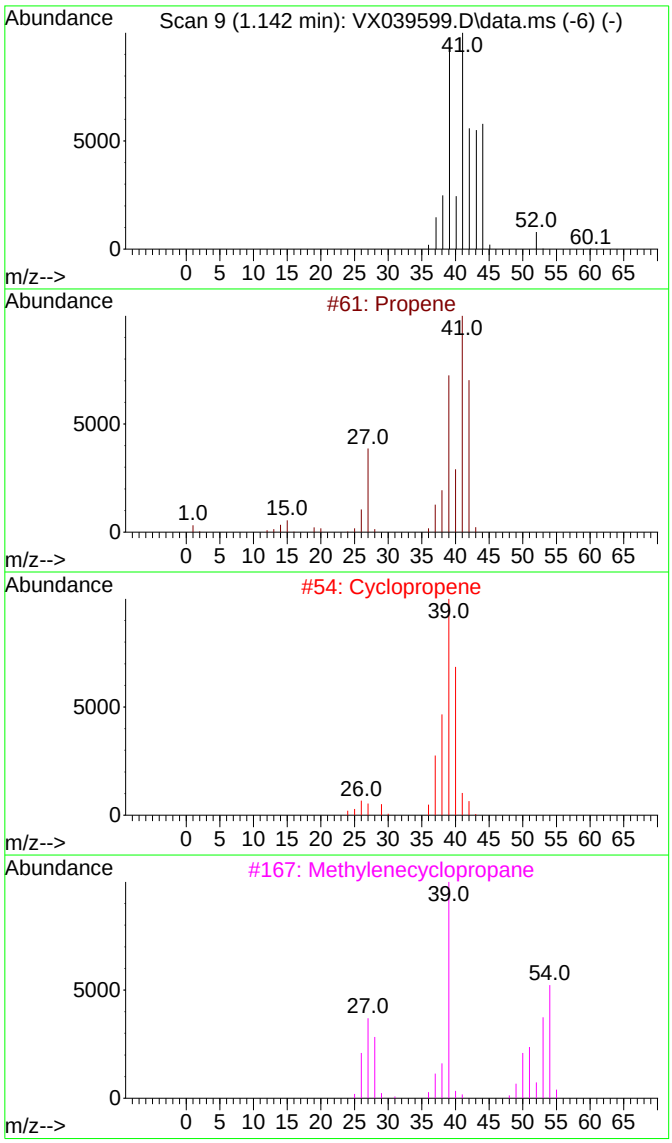
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

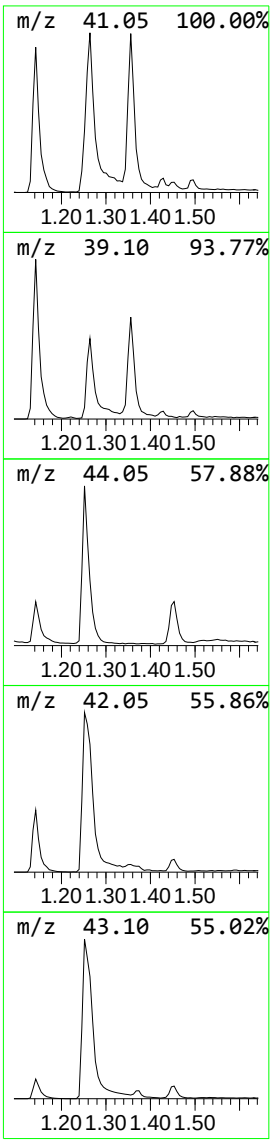
****

Peak Number 1 Propene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	32.83 ug/l	181753	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	86
2	Cyclopropene	40	C3H4	002781-85-3	9
3	Methylenecyclopropane	54	C4H6	006142-73-0	4
4	Cyclopropane	42	C3H6	000075-19-4	4
5	2-Oxetanone, 4-methyl-	86	C4H6O2	003068-88-0	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039599.D
Acq On : 03 Jan 2024 14:05
Operator : JC/MD
Sample : P1002-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1211

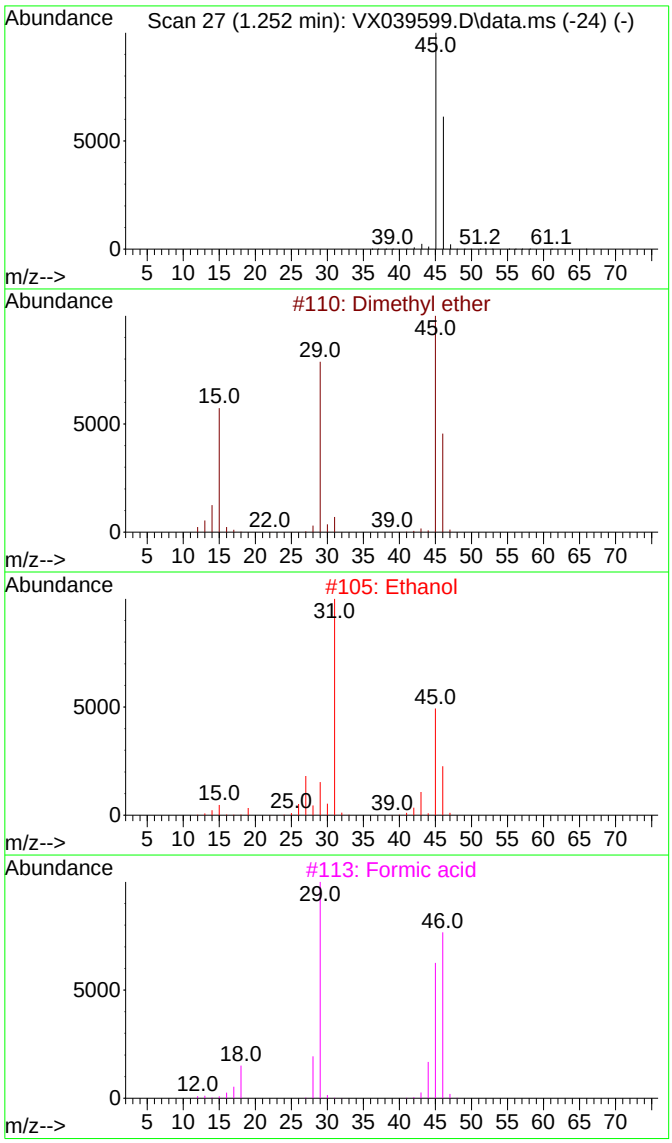
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

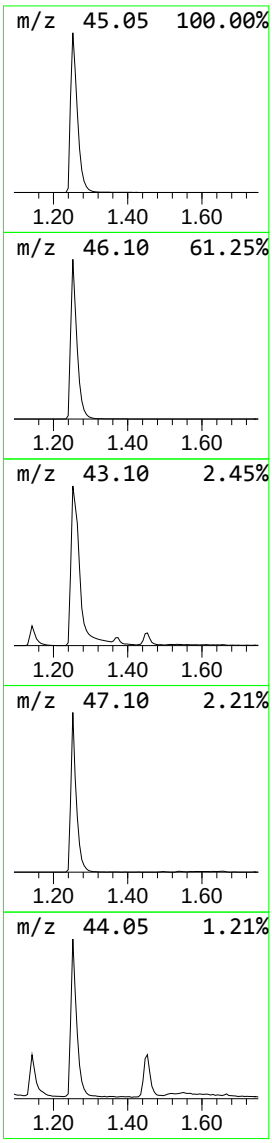
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Dimethyl ether Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	2598.49 ug/l	14386500	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 : VX039599.D
Acq On : 03 Jan 2024 14:05
Operator : JC/MD
Sample : P1002-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1211

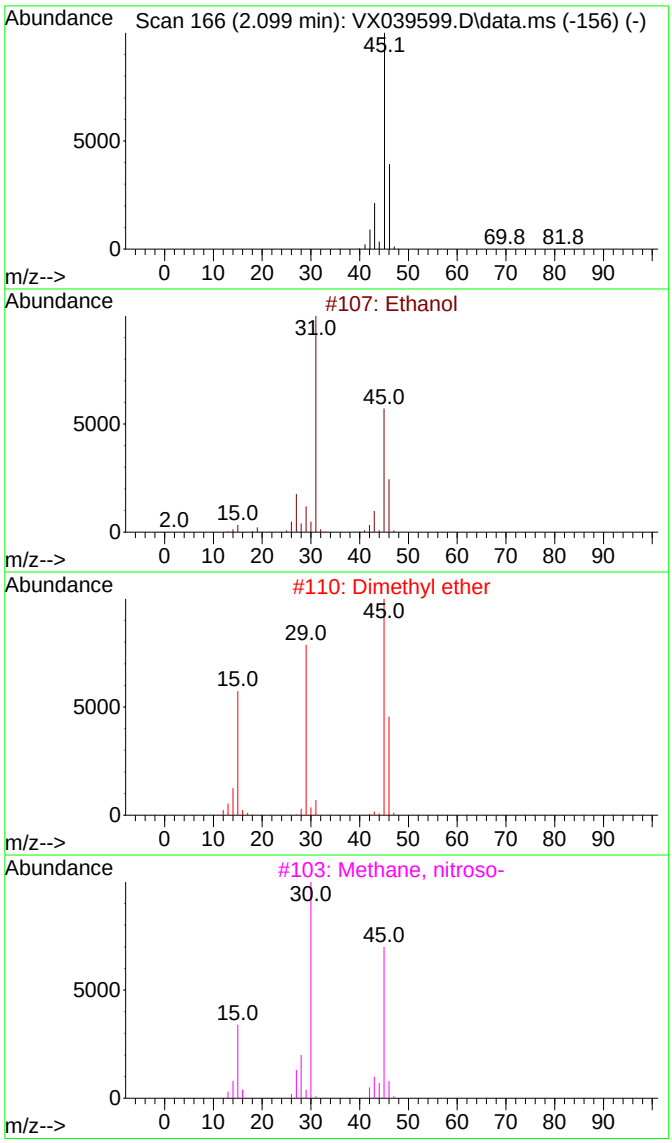
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

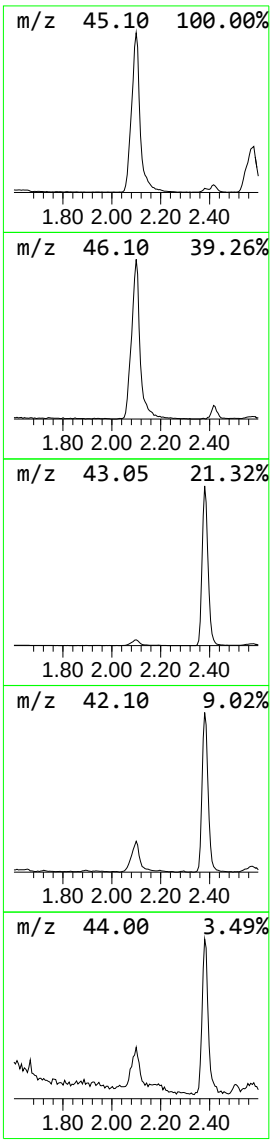
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.099	56.27 ug/l	311534	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	Oxalic acid	90	C2H2O4	000144-62-7	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039599.D
Acq On : 03 Jan 2024 14:05
Operator : JC/MD
Sample : P1002-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1211

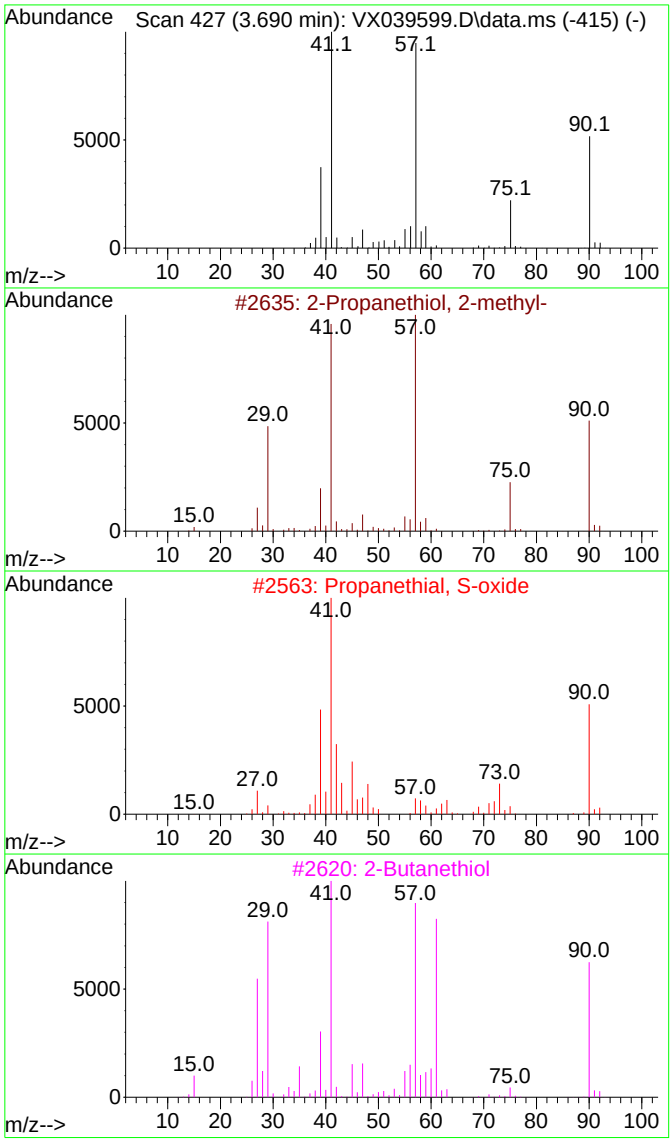
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

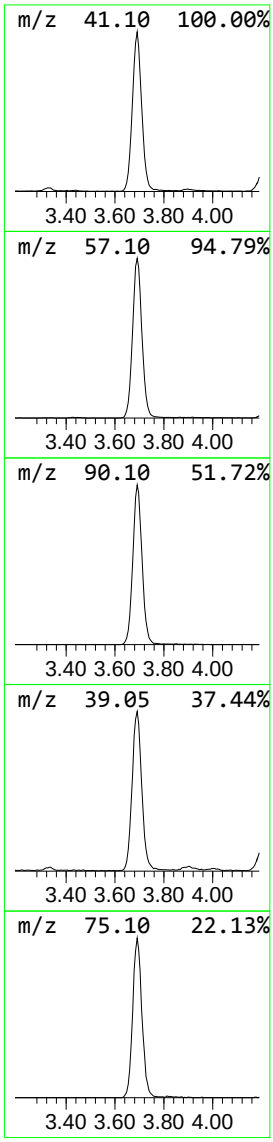
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Propanethiol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.690	183.07 ug/l	1013550	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol, 2-methyl-	90	C4H10S	000075-66-1	91
2	Propanethial, S-oxide	90	C3H6OS	032157-29-2	38
3	2-Butanethiol	90	C4H10S	000513-53-1	36
4	Propane, 2-chloro-2-methyl-	92	C4H9Cl	000507-20-0	16
5	Butanal, 2-methyl-	86	C5H10O	000096-17-3	16





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039599.D
Acq On : 03 Jan 2024 14:05
Operator : JC/MD
Sample : P1002-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1211

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

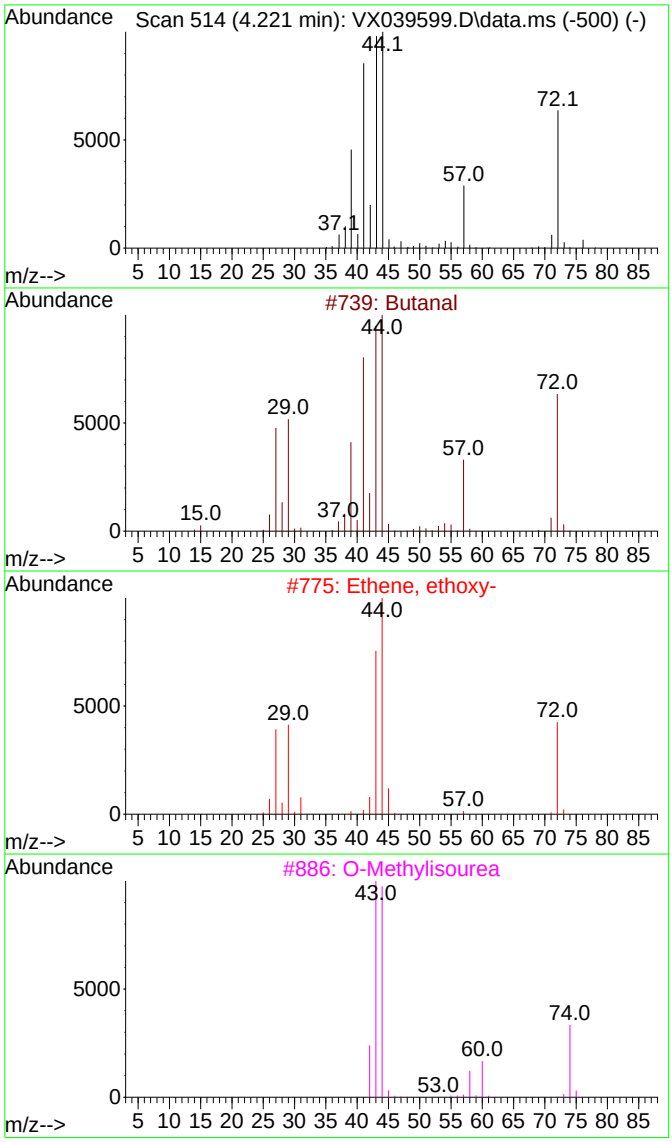
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

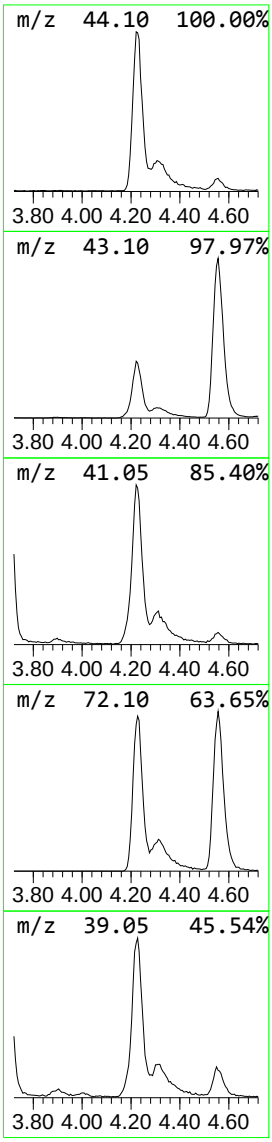
****

Peak Number 5 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.221	120.69 ug/l	668169	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	50
3	O-Methylisourea	74	C2H6N2O	002440-60-0	42
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	30
5	1,3-Butanediol, (S)-	90	C4H10O2	024621-61-2	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039599.D
Acq On : 03 Jan 2024 14:05
Operator : JC/MD
Sample : P1002-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1211

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

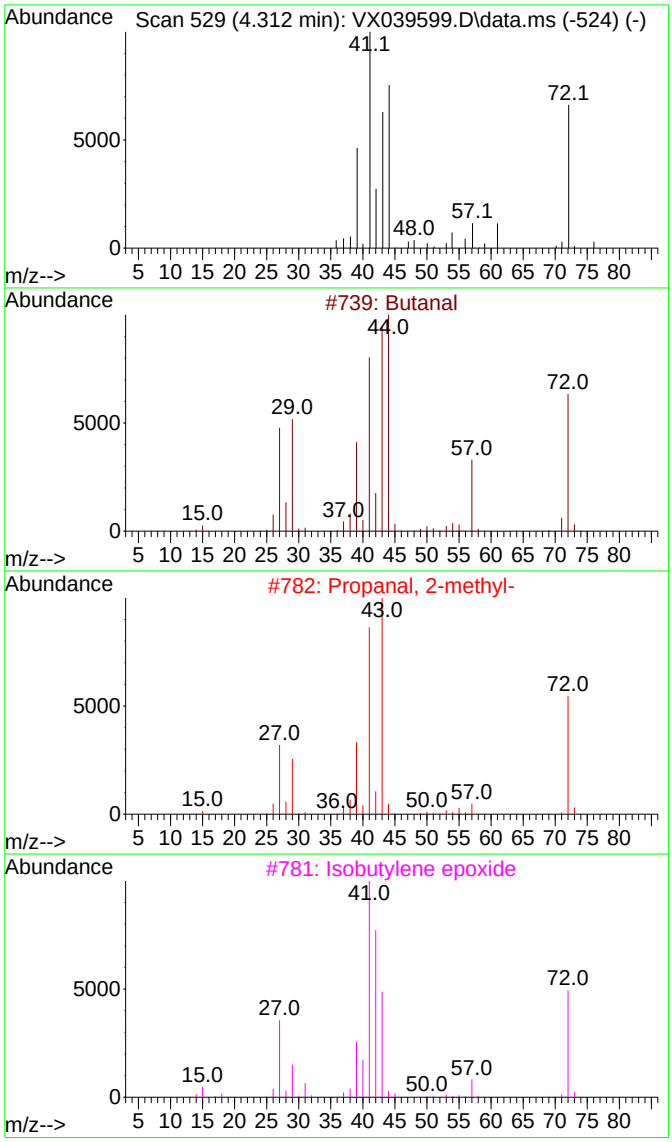
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

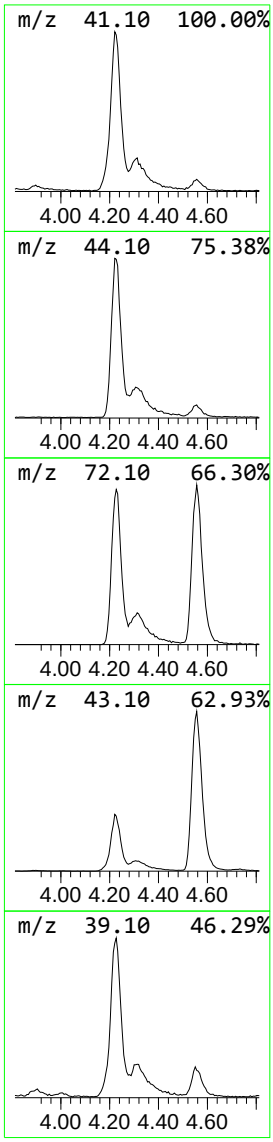
****

Peak Number 6 unknown4.312 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.312	35.14 ug/l	194558	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	52
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
3	Isobutylene epoxide	72	C4H8O	000558-30-5	10
4	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	9
5	Silacyclobutane	72	C3H8Si	1000434-34-1	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039599.D
Acq On : 03 Jan 2024 14:05
Operator : JC/MD
Sample : P1002-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1211

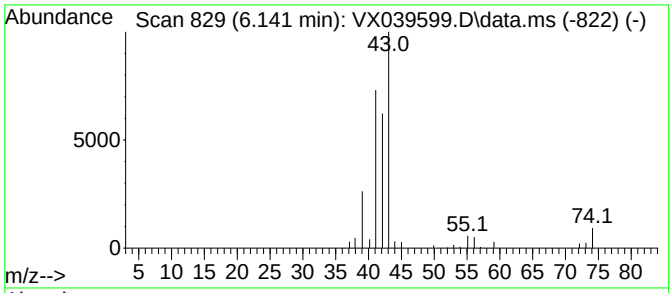
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

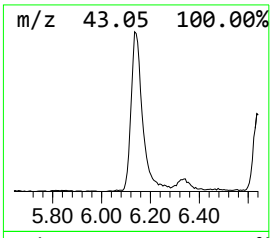
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

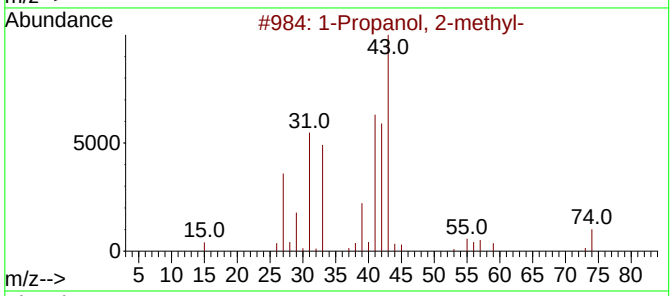
****
Peak Number 7 1-Propanol, 2-methyl- Concentration Rank 7

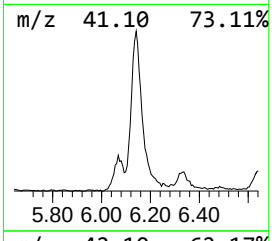
R.T.	EstConc	Area	Relative to ISTD	R.T.
6.141	35.93 ug/l	198936	Pentafluorobenzene	5.550

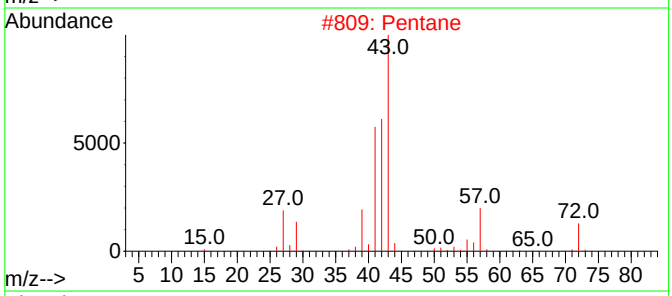
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	90
2	Pentane	72	C5H12	000109-66-0	39
3	Isobutylene epoxide	72	C4H8O	000558-30-5	28
4	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	28
5	Propanal, 2-methyl-	72	C4H8O	000078-84-2	27

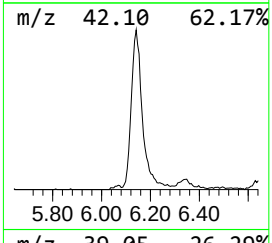


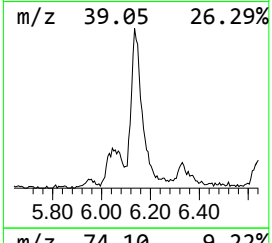


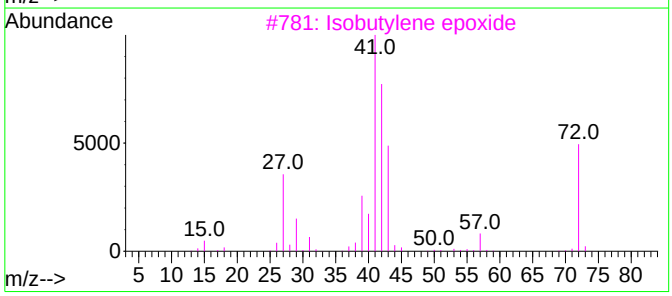


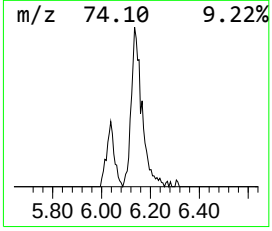












Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039599.D
Acq On : 03 Jan 2024 14:05
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Sample : P1002-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1211

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

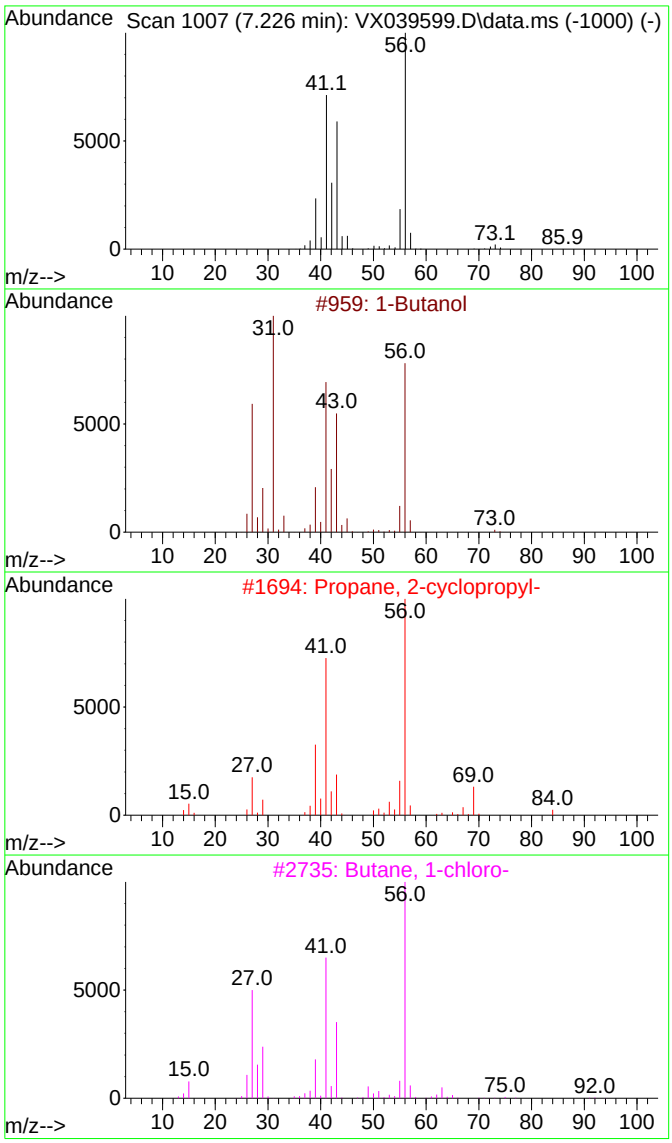
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

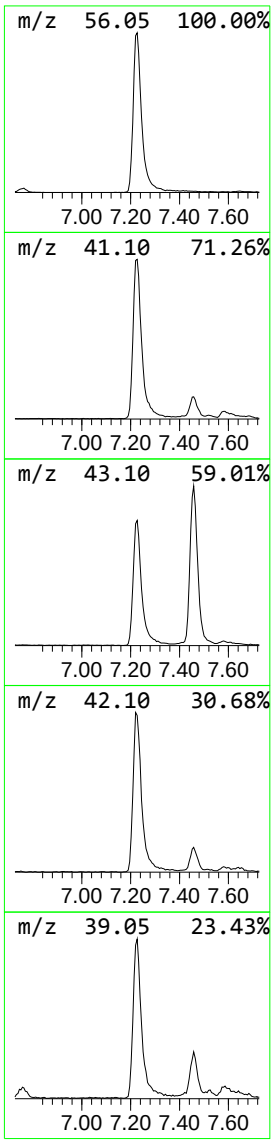
****

Peak Number 8 1-Butanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.226	78.53 ug/l	694235	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	86
2	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	36
3	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9
4	Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
5	Oxetane, 2,3,4-trimethyl-, (2.al...	100	C6H12O	032347-12-9	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039599.D
Acq On : 03 Jan 2024 14:05
Operator : JC/MD
Sample : P1002-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1211

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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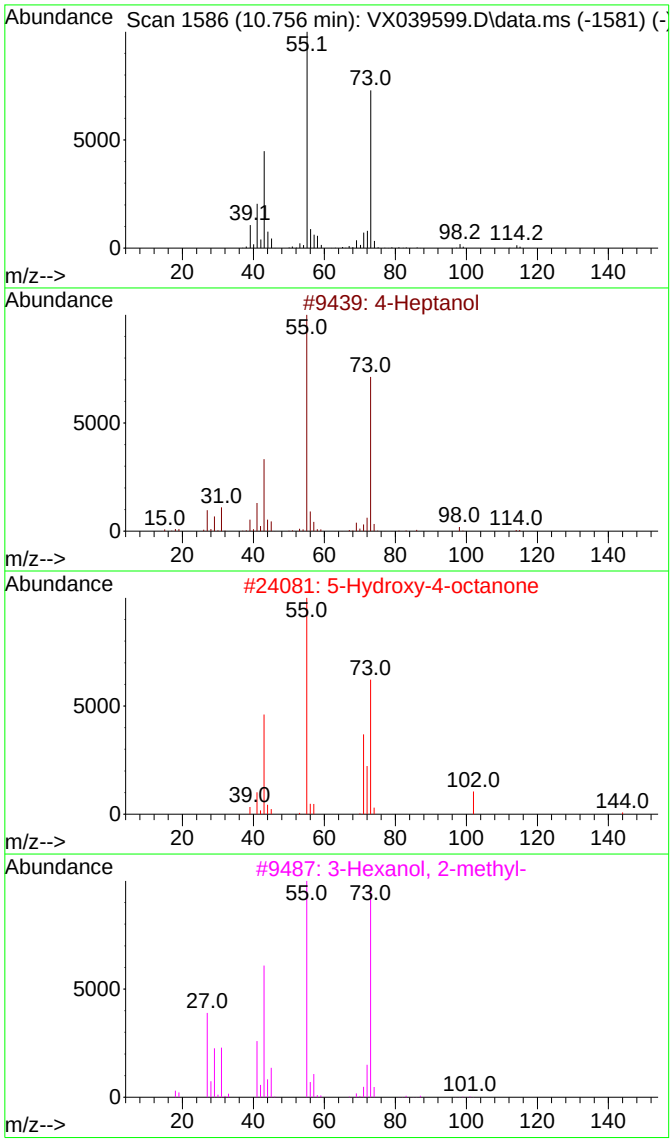
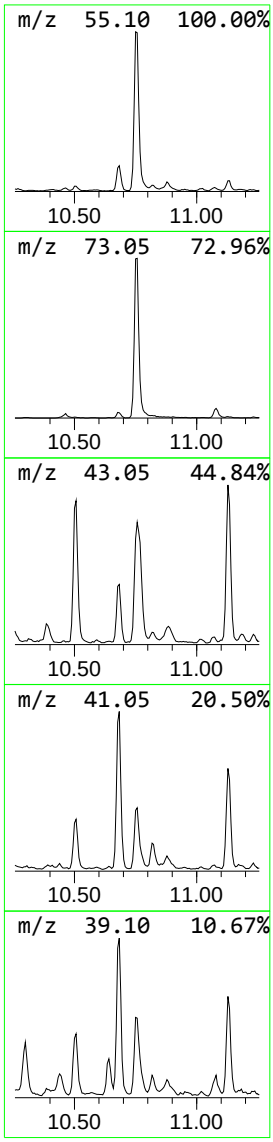
Peak Number 9 4-Heptanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.756	33.57 ug/l	438918	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol	116	C7H16O	000589-55-9	64
2	5-Hydroxy-4-octanone	144	C8H16O2	000496-77-5	37
3	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	37
4	4,5-Octanediol	146	C8H18O2	022607-10-9	28
5	2-Propenoic acid, 2-hydroxyethyl...	116	C5H8O3	000818-61-1	28





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039599.D
Acq On : 03 Jan 2024 14:05
Operator : JC/MD
Sample : P1002-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1211

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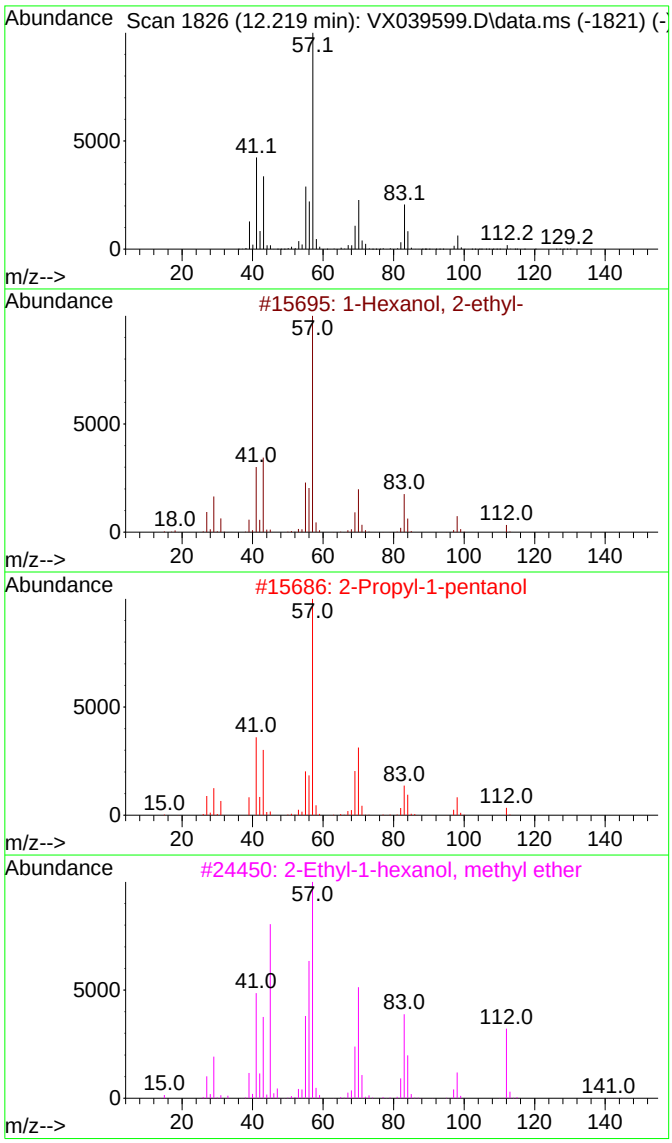
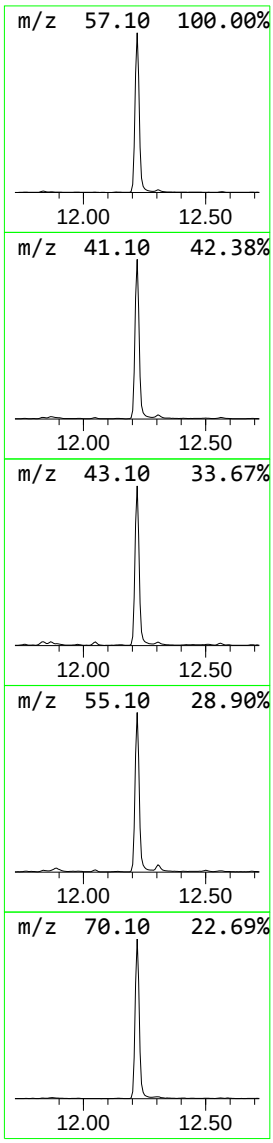
Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	643.85 ug/l	7492780	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	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
4	1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	47
5	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039599.D
Acq On : 03 Jan 2024 14:05
Operator : JC/MD
Sample : P1002-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
1211

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
Propene	1.142	32.8	ug/l	181753	1	5.550	276824	50.0
Dimethyl ether	1.252	2598.5	ug/l	14386500	1	5.550	276824	50.0
Ethanol	2.099	56.3	ug/l	311534	1	5.550	276824	50.0
2-Propanethiol,...	3.690	183.1	ug/l	1013550	1	5.550	276824	50.0
Butanal	4.221	120.7	ug/l	668169	1	5.550	276824	50.0
unknown4.312	4.312	35.1	ug/l	194558	1	5.550	276824	50.0
1-Propanol, 2-m...	6.141	35.9	ug/l	198936	1	5.550	276824	50.0
1-Butanol	7.226	78.5	ug/l	694235	2	6.757	442021	50.0
4-Heptanol	10.756	33.6	ug/l	438918	3	10.055	653764	50.0
1-Hexanol, 2-et...	12.219	643.9	ug/l	7492780	4	12.024	581872	50.0