LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039593.D
Acq On : 03 Jan 2024 11:49
Operator : JC/MD
Sample : P1001-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1205

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: VX039593.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.447	55	59	69	rBV	4737394	6057743	100.00%	37.470%
2	1.538	69	74	97	rVV	365298	1457592	24.06%	9.016%
3	1.691	97	99	130	rVB	36099	138654	2.29%	0.858%
4	2.117	158	169	180	rVB	80790	206840	3.41%	1.279%
5	2.386	206	213	227	rVB	54985	100259	1.66%	0.620%
6	4.227	502	515	524	rBV	444483	1219011	20.12%	7.540%
7	4.324	524	531	559	rVV2	92747	440343	7.27%	2.724%
8	4.562	562	570	586	rVB2	22671	74925	1.24%	0.463%
9	5.385	694	705	720	rVB2	63506	189971	3.14%	1.175%
10	5.544	720	731	746	rBV	96460	272641	4.50%	1.686%
11	5.952	789	798	818	rBV	75611	204738	3.38%	1.266%
12	6.757	920	930	944	rBV	182988	436423	7.20%	2.699%
13	7.232	1000	1008	1029	rBV	112830	268625	4.43%	1.662%
14	7.580	1059	1065	1069	rBV	49721	108335	1.79%	0.670%
15	8.647	1233	1240	1248	rBV	387797	602496	9.95%	3.727%
16	10.055	1464	1471	1483	rBV	412367	602210	9.94%	3.725%
17	10.756	1581	1586	1595	rBV	122830	185928	3.07%	1.150%
18	11.079	1634	1639	1645	rBV	351112	453986	7.49%	2.808%
19	11.421	1692	1695	1705	rVB	118830	153360	2.53%	0.949%
20	11.573	1715	1720	1723	rBV2	50035	67889	1.12%	0.420%
21	11.603	1723	1725	1733	rVV	49441	66312	1.09%	0.410%
22	11.683	1733	1738	1746	rVB	104463	124710	2.06%	0.771%
23	11.988	1783	1788	1790	rBV	299940	348982	5.76%	2.159%
24	12.018	1790	1793	1802	rVB	427061	588989	9.72%	3.643%
25	12.219	1820	1826	1837	rBV	1215372	1630493	26.92%	10.085%
26	12.305	1837	1840	1851	rVB5	32072	69861	1.15%	0.432%
27	13.676	2060	2065	2070	rVB	81963	95708	1.58%	0.592%

Sum of corrected areas: 16167024

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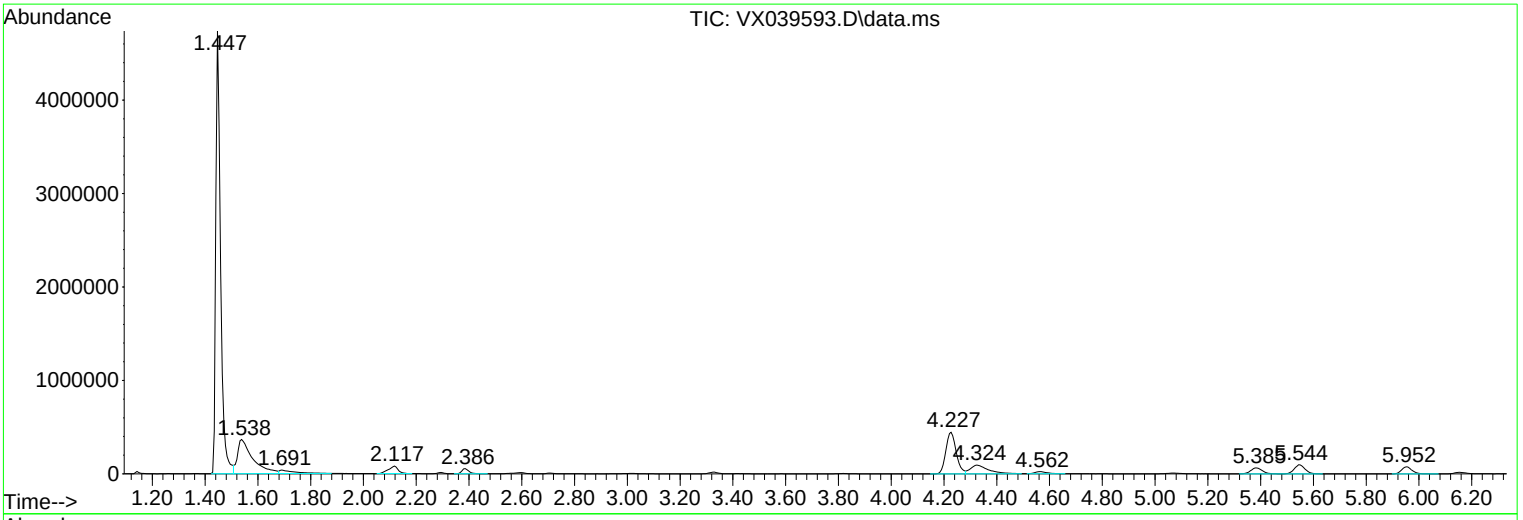
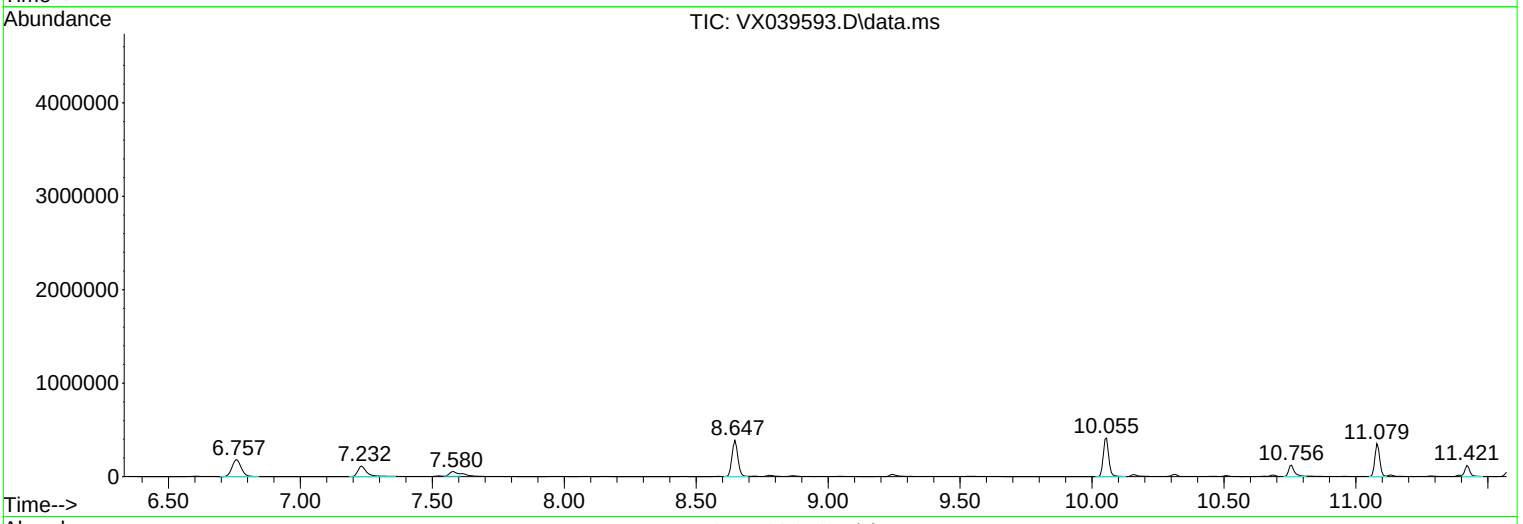
ALS Vial : 7 Sample Multiplier: 1

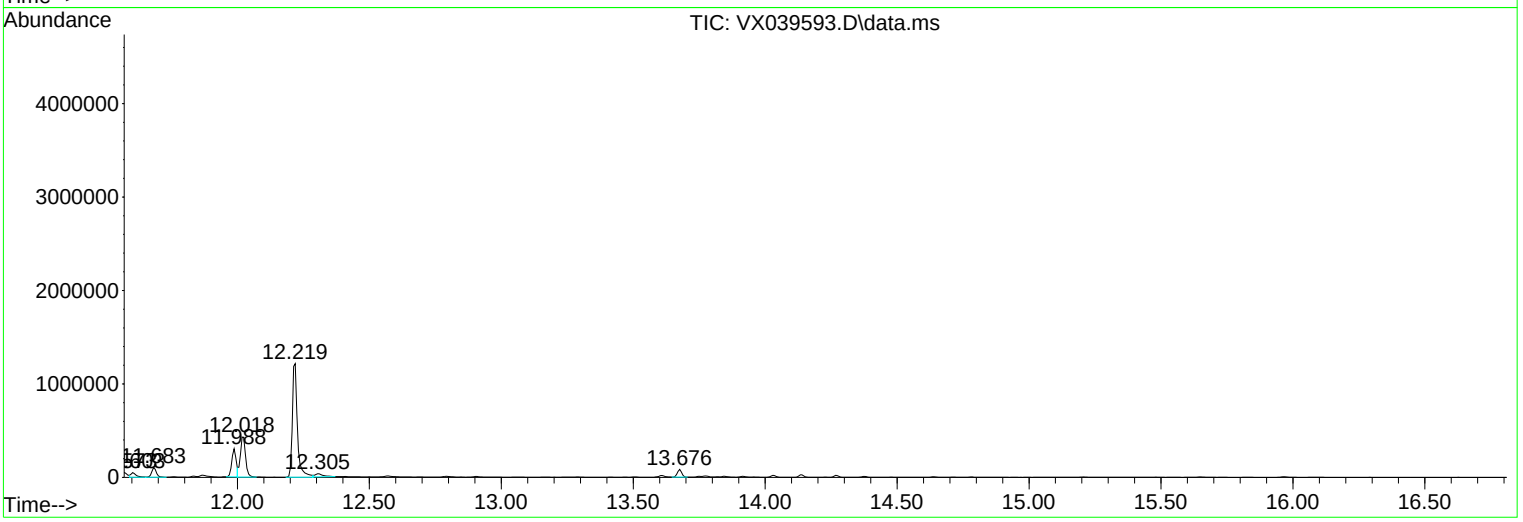
Instrument :
MSVOA_X
ClientSampleId :
ORA-1205

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 : VX039593.D
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Quant Title : SW846 8260

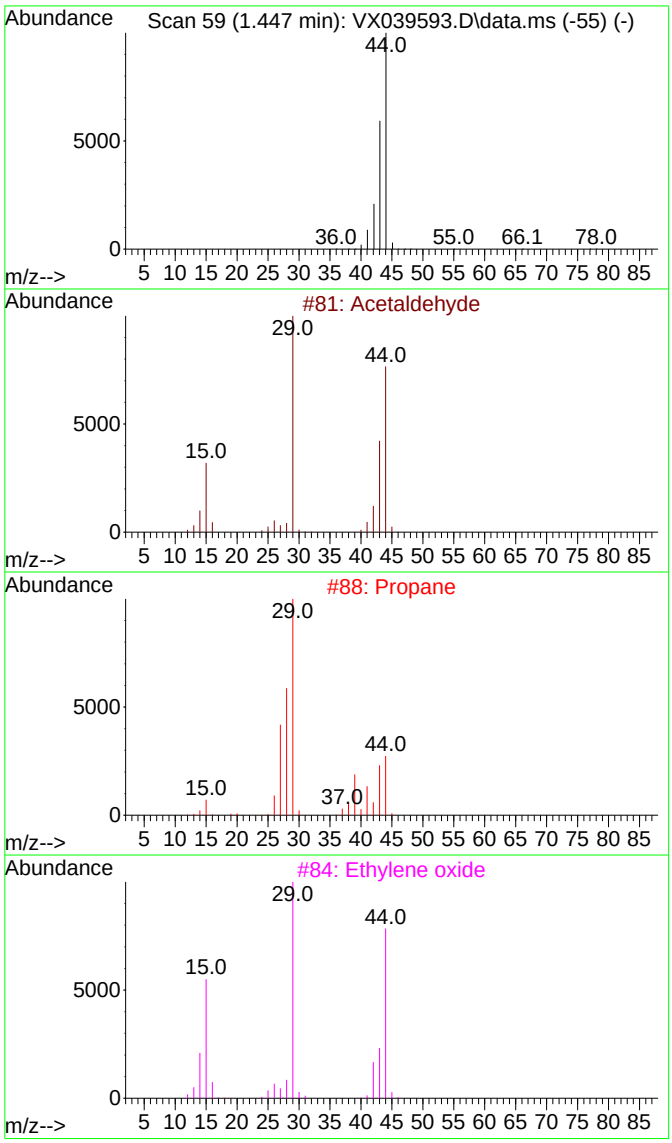
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

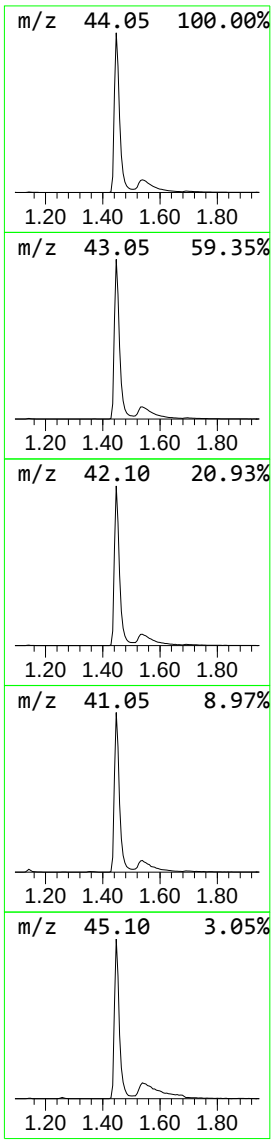
****

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.447	1110.94 ug/l	6057740	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	74
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Alanine	89	C3H7NO2	000056-41-7	4
5	Hydrogen isocyanate	43	CHNO	000075-13-8	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039593.D
Acq On : 03 Jan 2024 11:49
Operator : JC/MD
Sample : P1001-01
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1205

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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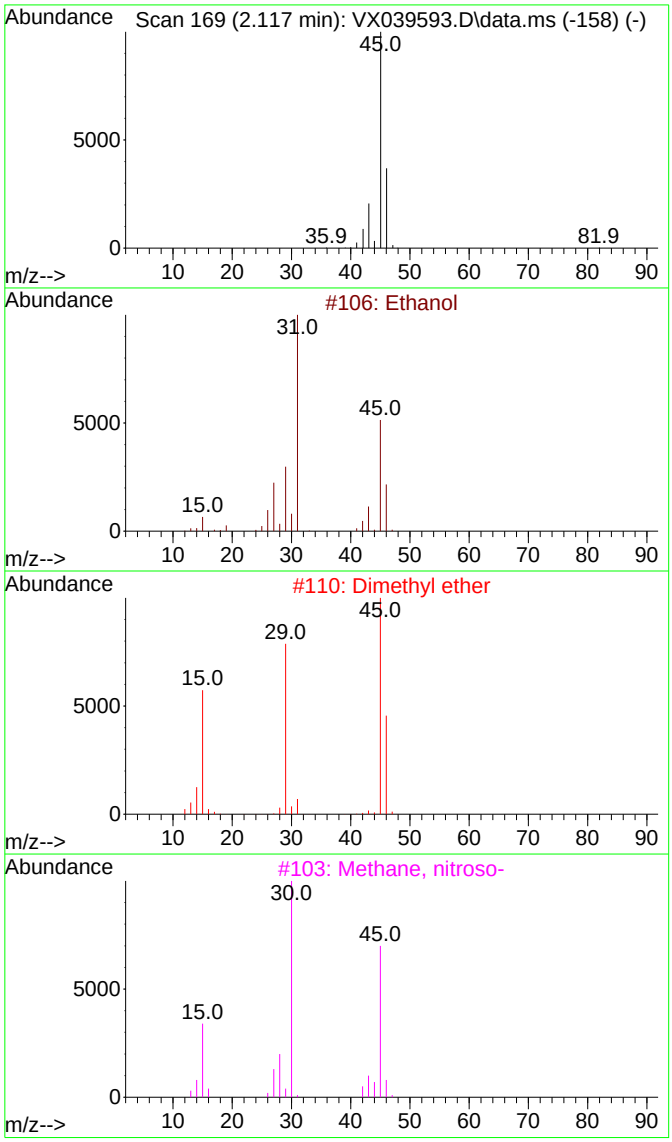
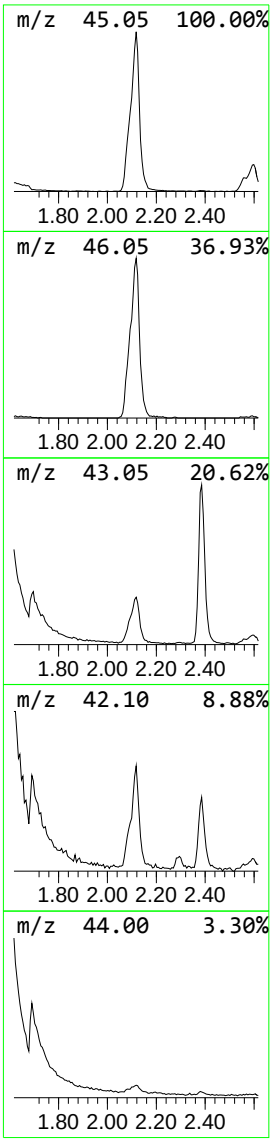
Peak Number 4 Ethanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.117	37.93 ug/l	206840	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	86
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	7
4	Formic acid	46	CH2O2	000064-18-6	4
5	Formamide	45	CH3NO	000075-12-7	2





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Data File : VX039593.D
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Operator : JC/MD
Sample : P1001-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1205

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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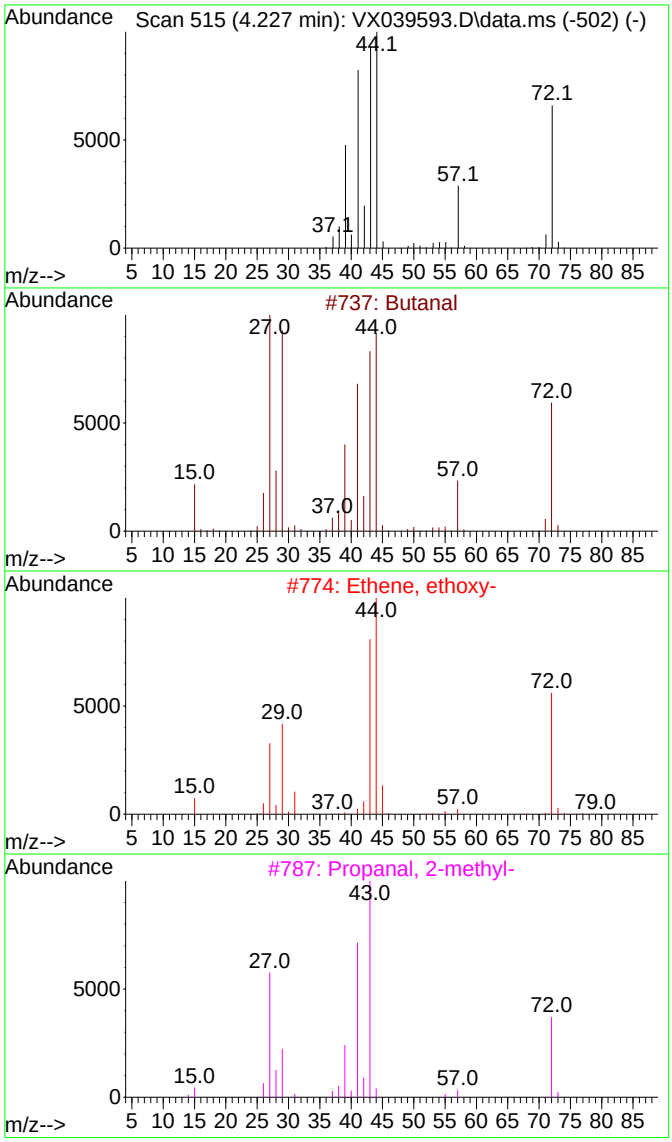
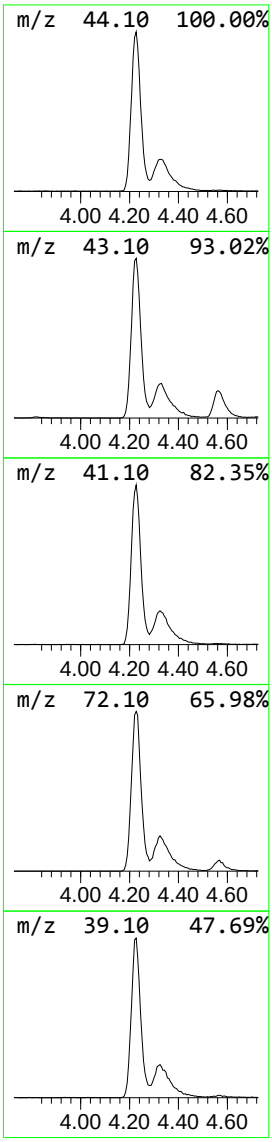
Peak Number 5 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	223.56 ug/l	1219010	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Ethene, ethoxy-	72	C4H8O	000109-92-2	47
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	38
4	Methacrolein	70	C4H6O	000078-85-3	27
5	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	25





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039593.D
Acq On : 03 Jan 2024 11:49
Operator : JC/MD
Sample : P1001-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1205

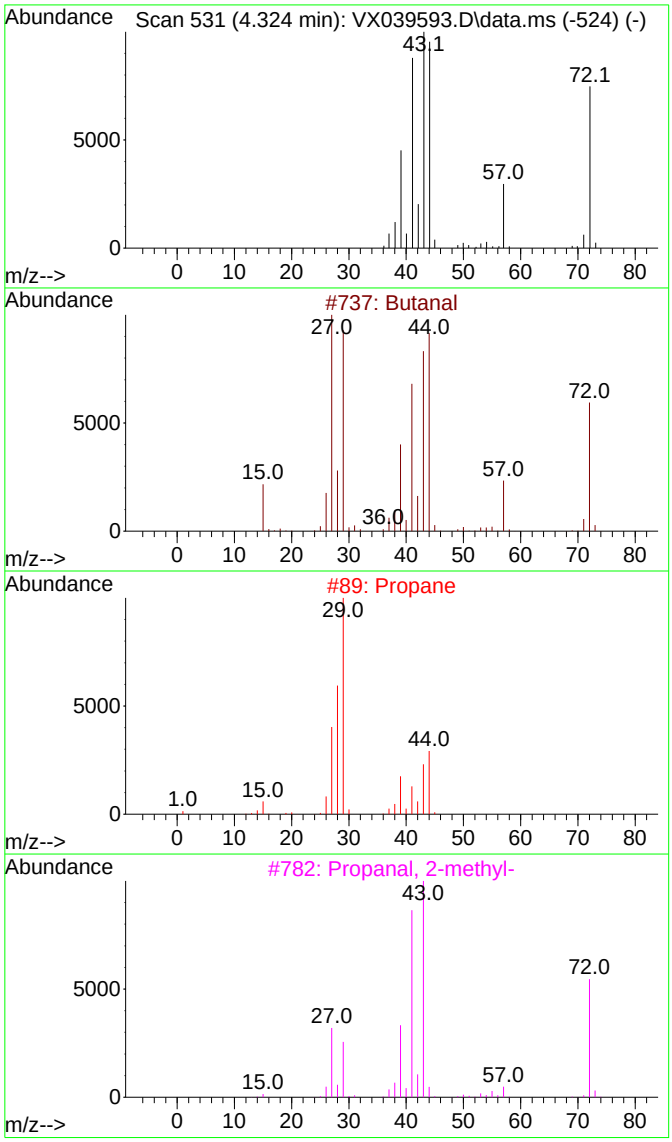
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

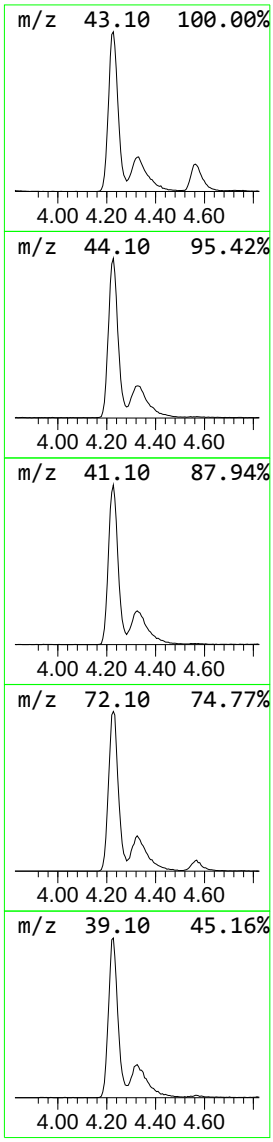
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Propane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.324	80.76 ug/l	440343	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	50
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	47
4	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37
5	Isobutylene epoxide	72	C4H8O	000558-30-5	16





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Operator : JC/MD
Sample : P1001-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1205

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

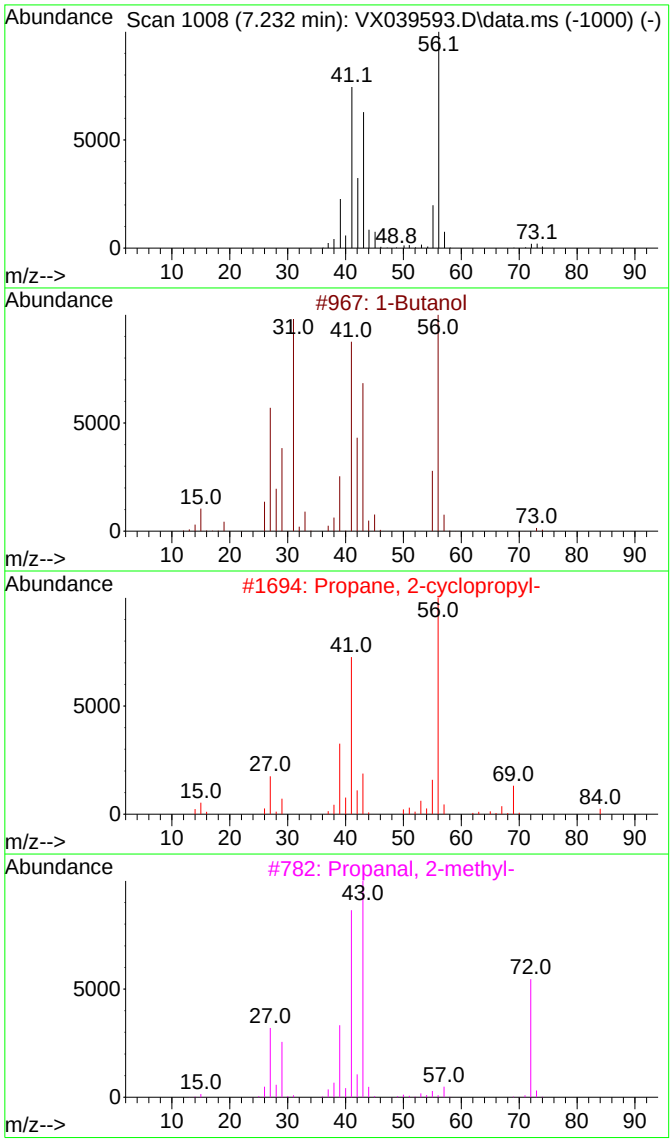
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

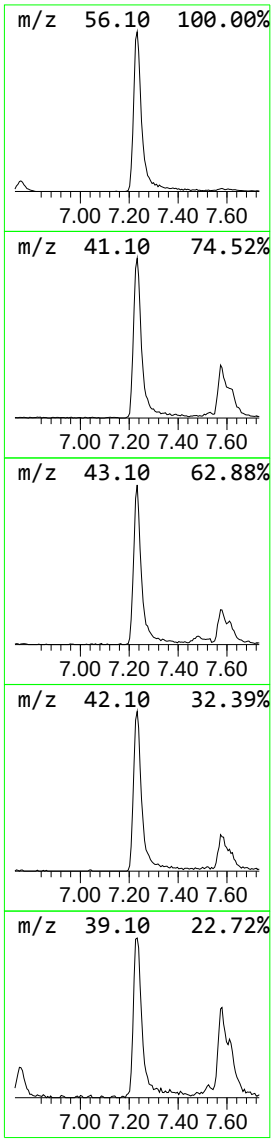
****

Peak Number 7 1-Butanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.232	30.78 ug/l	268625	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	90
2	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	39
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	10
4	Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
5	Neopentyl glycol	104	C5H12O2	000126-30-7	9





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1205

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

TIC Library : C:\Database\NIST20.L
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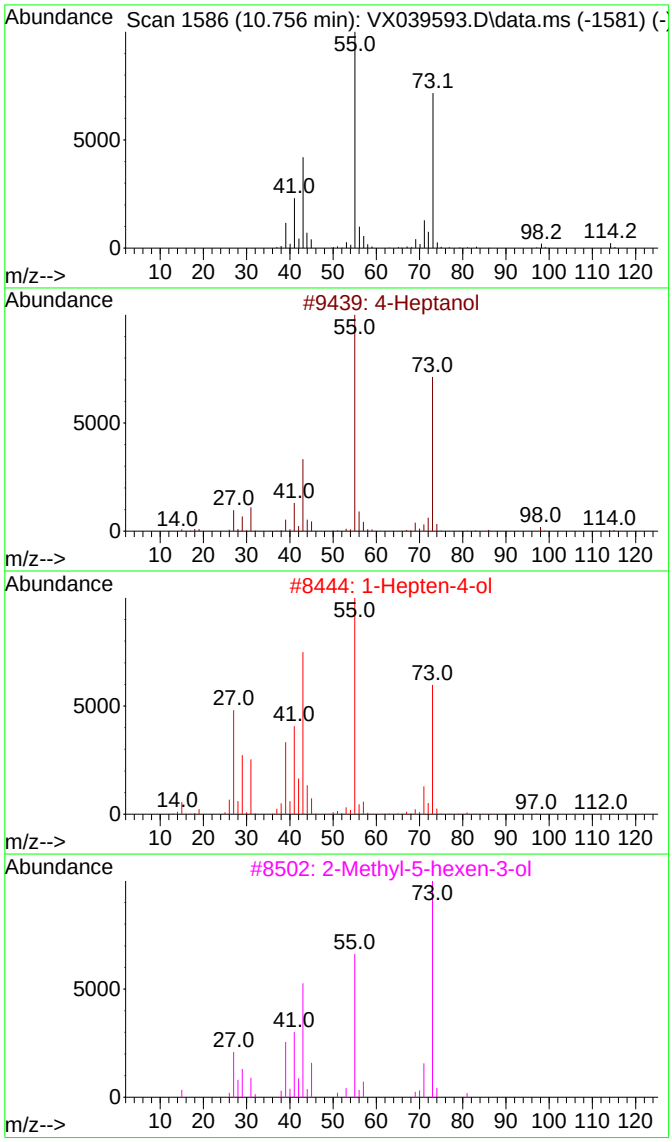
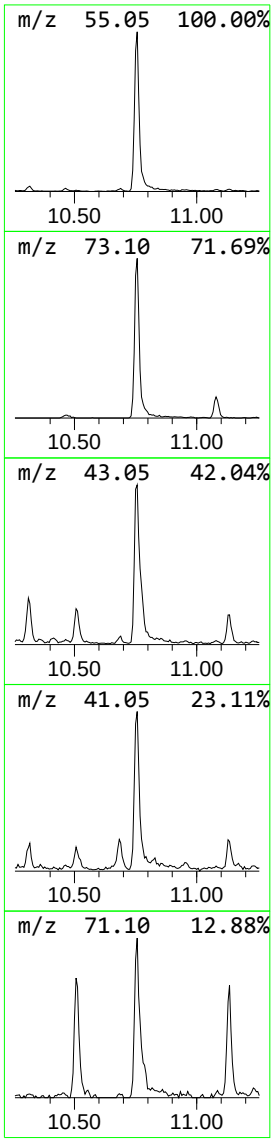
****
Peak Number 8 4-Heptanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.756	15.44 ug/l	185928	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol	116	C7H16O	000589-55-9	72
2	1-Hepten-4-ol	114	C7H14O	003521-91-3	50
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
4	4-Decanol	158	C10H22O	002051-31-2	36
5	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	36





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MSVOA_X
ClientSampleId :
ORA-1205

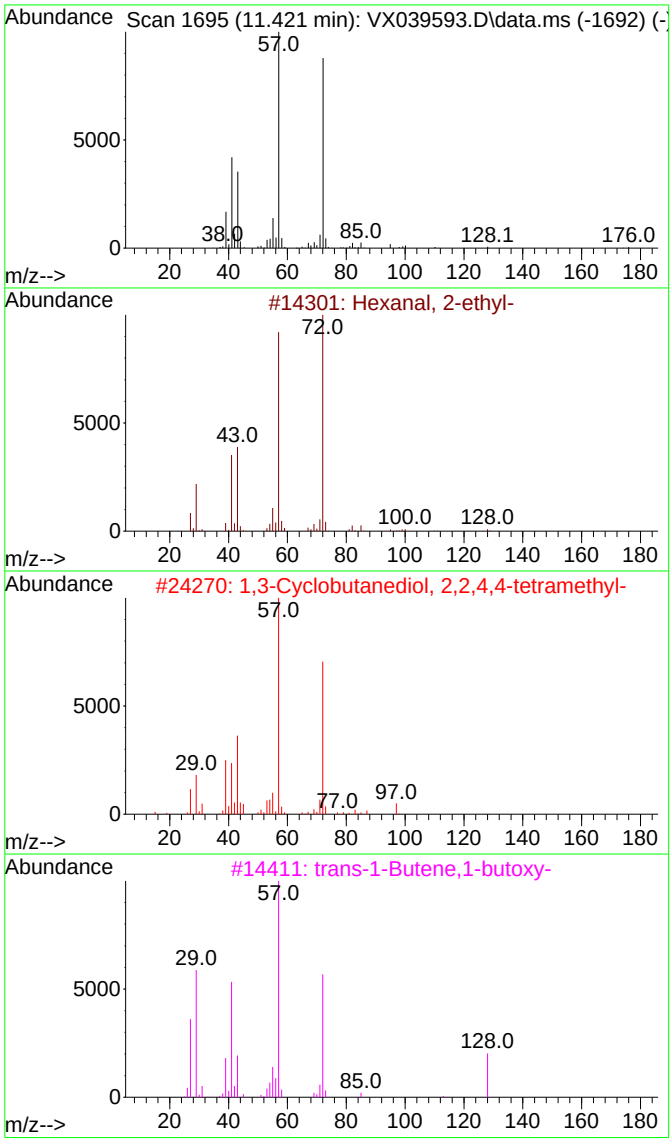
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

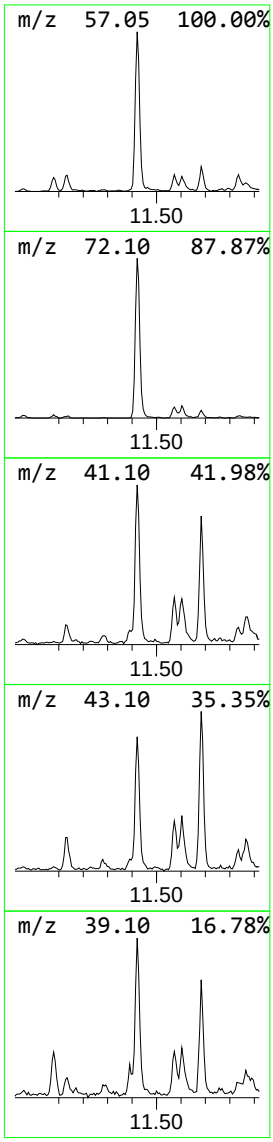
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Hexanal, 2-ethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.421	13.02 ug/l	153360	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	90
2	1,3-Cyclobutanediol, 2,2,4,4-tet...	144	C8H16O2	003010-96-6	56
3	trans-1-Butene,1-butoxy-	128	C8H16O	1000139-52-8	56
4	Pentane, 1-(1-butenyloxy)-, (Z)-	142	C9H18O	056052-76-7	45
5	1-Hexanamine, N-propyl-	143	C9H21N	020193-23-1	42





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MSVOA_X
ClientSampleId :
ORA-1205

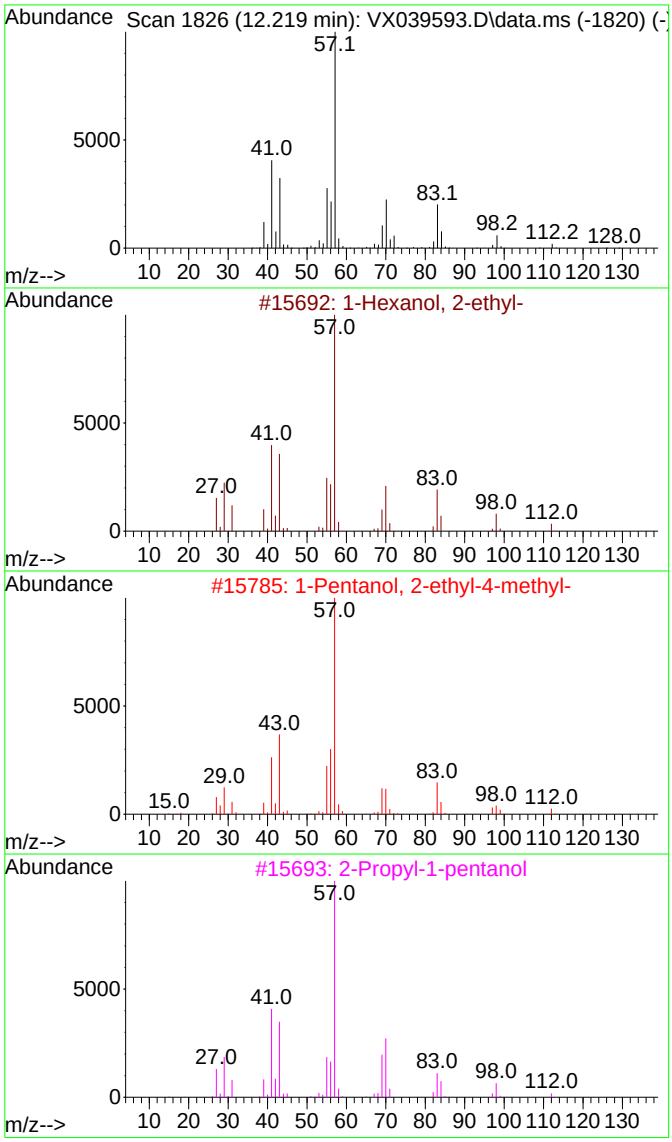
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

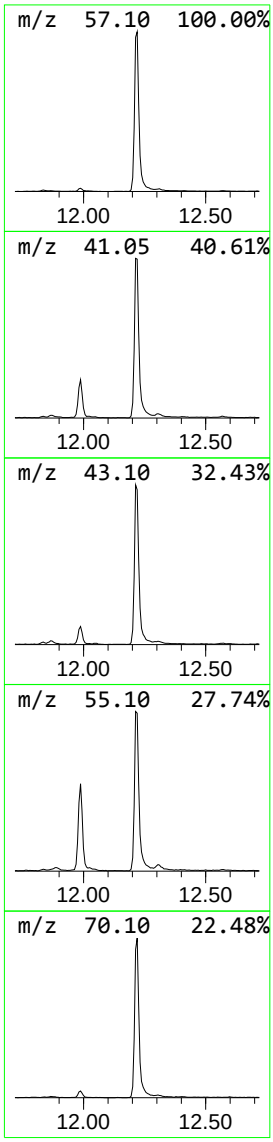
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	138.41 ug/l	1630490	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-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
4	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
5	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	42





Tentatively Identified Compound (LSC) summary

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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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Acetaldehyde	1.447	1110.9	ug/l	6057740	1	5.550	272641	50.0
Ethanol	2.117	37.9	ug/l	206840	1	5.550	272641	50.0
Butanal	4.227	223.6	ug/l	1219010	1	5.550	272641	50.0
Propane	4.324	80.8	ug/l	440343	1	5.550	272641	50.0
1-Butanol	7.232	30.8	ug/l	268625	2	6.757	436423	50.0
4-Heptanol	10.756	15.4	ug/l	185928	3	10.055	602210	50.0
Hexanal, 2-ethyl-	11.421	13.0	ug/l	153360	4	12.024	588989	50.0
1-Hexanol, 2-et...	12.219	138.4	ug/l	1630490	4	12.024	588989	50.0