LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039594.D
Acq On : 03 Jan 2024 12:12
Operator : JC/MD
Sample : P1001-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1206

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: VX039594.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	67	rBV	2322187	2873507	100.00%	24.339%
2	1.514	67	70	115	rVB	147857	583641	20.31%	4.944%
3	2.099	157	166	184	rVB	45699	102993	3.58%	0.872%
4	2.379	205	212	223	rVB	40961	73671	2.56%	0.624%
5	4.227	503	515	523	rBV	282919	766419	26.67%	6.492%
6	4.300	523	527	555	rVB2	49201	185450	6.45%	1.571%
7	4.562	563	570	586	rVB2	17306	52954	1.84%	0.449%
8	5.385	693	705	722	rBV	74633	217858	7.58%	1.845%
9	5.550	722	732	749	rVV2	105246	305628	10.64%	2.589%
10	5.952	788	798	814	rBV	84978	229752	8.00%	1.946%
11	6.147	822	830	840	rBV4	12528	37464	1.30%	0.317%
12	6.757	920	930	946	rBV	204688	488734	17.01%	4.140%
13	7.226	999	1007	1029	rBV	106105	255909	8.91%	2.168%
14	7.580	1060	1065	1087	rVB2	22065	67393	2.35%	0.571%
15	8.647	1234	1240	1249	rBV	439182	676086	23.53%	5.727%
16	9.244	1333	1338	1351	rBV	19149	38734	1.35%	0.328%
17	10.055	1465	1471	1484	rBV	459318	662617	23.06%	5.613%
18	10.756	1581	1586	1596	rBV	74631	118885	4.14%	1.007%
19	11.079	1634	1639	1645	rBV	391296	499002	17.37%	4.227%
20	11.420	1692	1695	1706	rVB	76019	101174	3.52%	0.857%
21	11.573	1714	1720	1722	rBV	36109	44707	1.56%	0.379%
22	11.603	1722	1725	1733	rVV	33904	52519	1.83%	0.445%
23	11.683	1733	1738	1744	rVV	170859	198833	6.92%	1.684%
24	11.865	1765	1768	1779	rVB3	16694	33634	1.17%	0.285%
25	11.987	1783	1788	1791	rVV	345133	451200	15.70%	3.822%
26	12.018	1791	1793	1802	rVB	459088	584159	20.33%	4.948%
27	12.219	1820	1826	1837	rBV	1404569	1836873	63.92%	15.559%
28	12.304	1837	1840	1852	rVB3	37050	75658	2.63%	0.641%
29	13.609	2047	2054	2060	rBV2	28143	43312	1.51%	0.367%
30	13.676	2060	2065	2070	rVB	88586	105537	3.67%	0.894%
31	14.139	2135	2141	2149	rVB	32063	41720	1.45%	0.353%

Sum of corrected areas: 11806023

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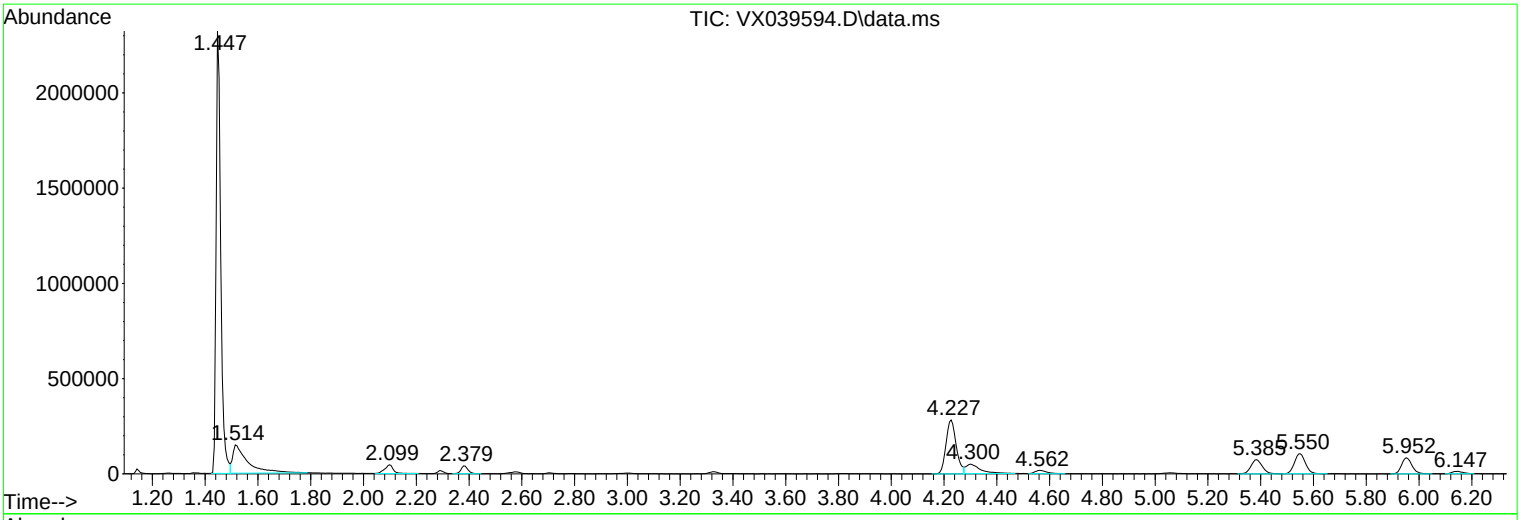
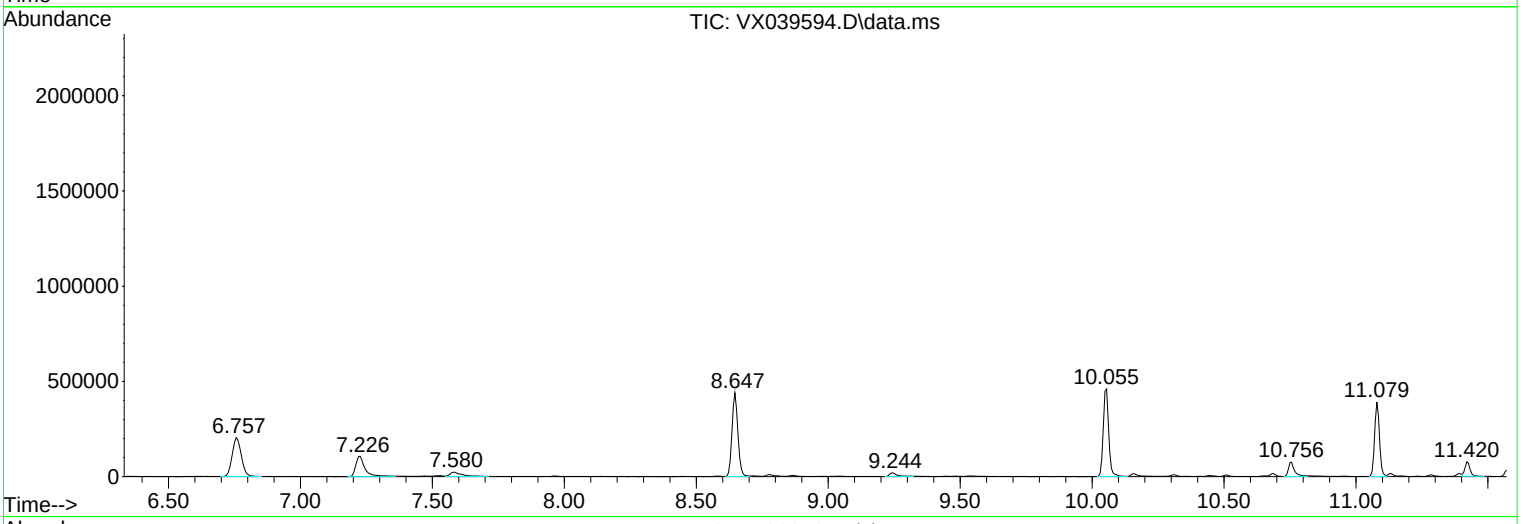
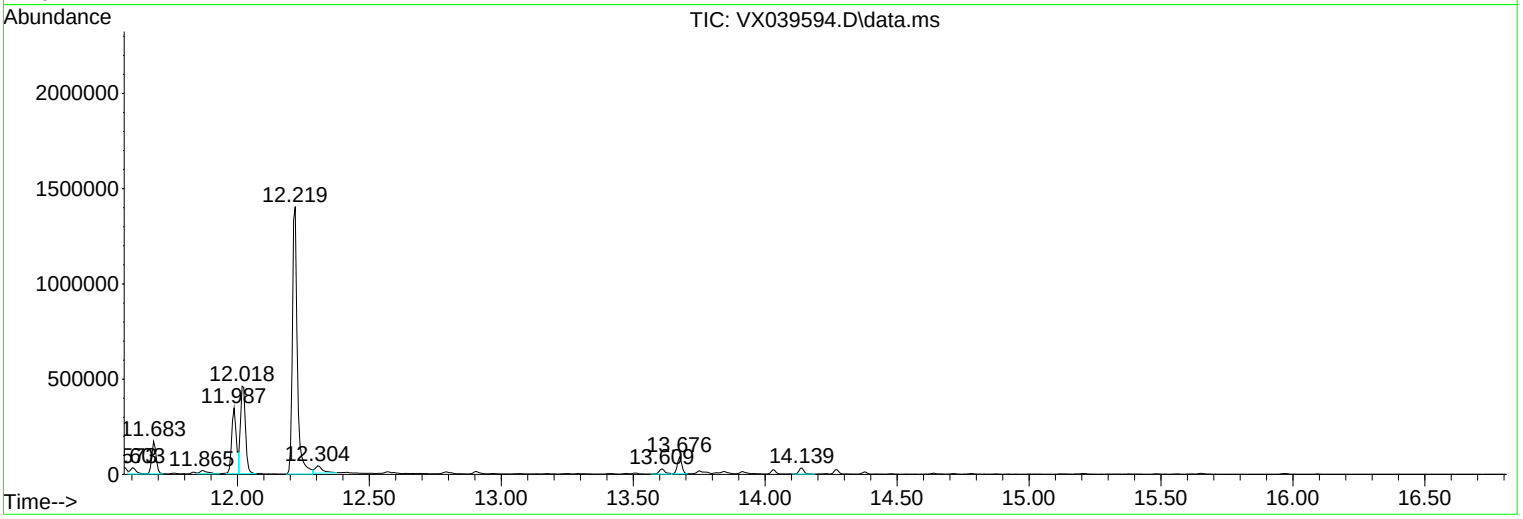
Instrument :
MSVOA_X
ClientSampleId :
ORA-1206

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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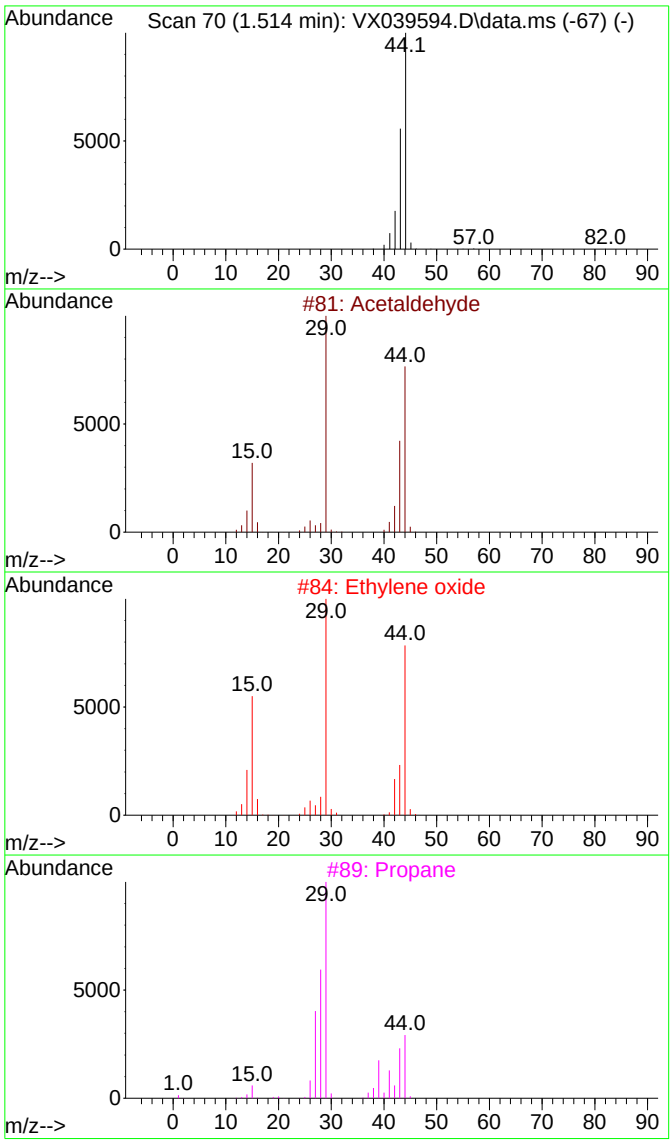
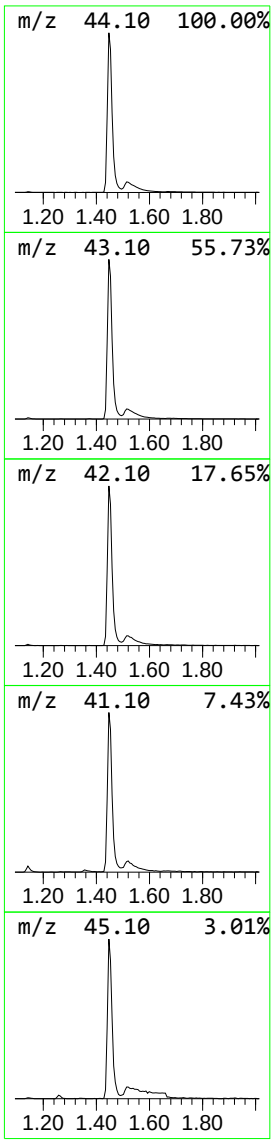
Peak Number 2 Acetaldehyde Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.514	95.48 ug/l	583641	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	64
2	Ethylene oxide	44	C2H4O	000075-21-8	5
3	Propane	44	C3H8	000074-98-6	4
4	Cyclopropyl carbinol	72	C4H8O	002516-33-8	4
5	1,2-Propanediamine	74	C3H10N2	000078-90-0	4





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ClientSampleId :
ORA-1206

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
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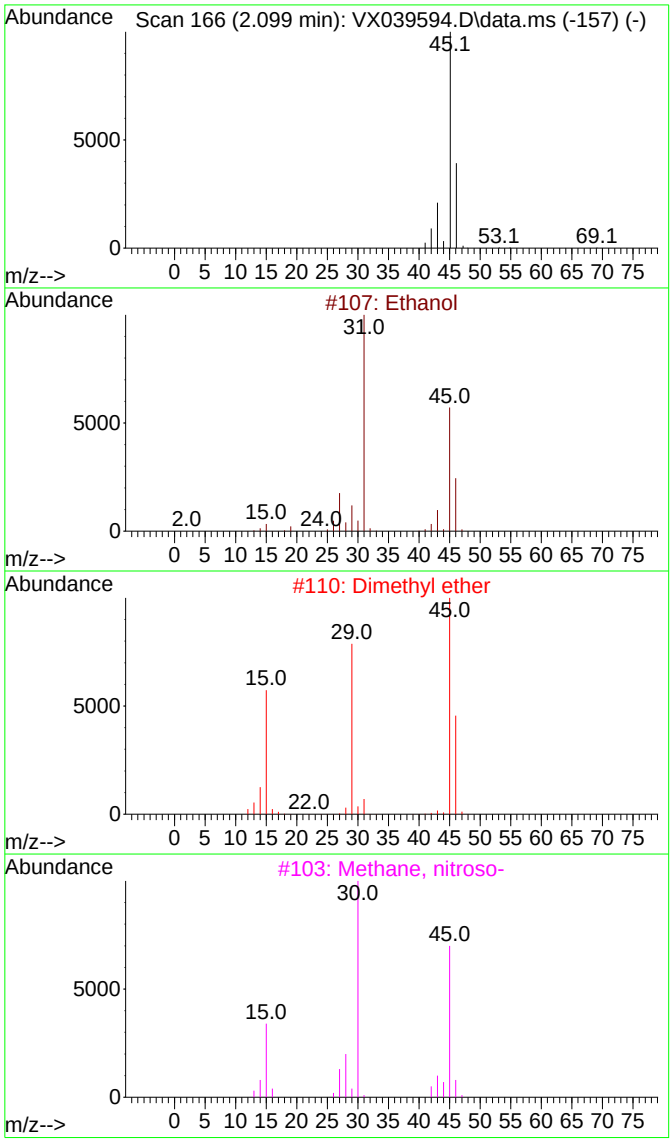
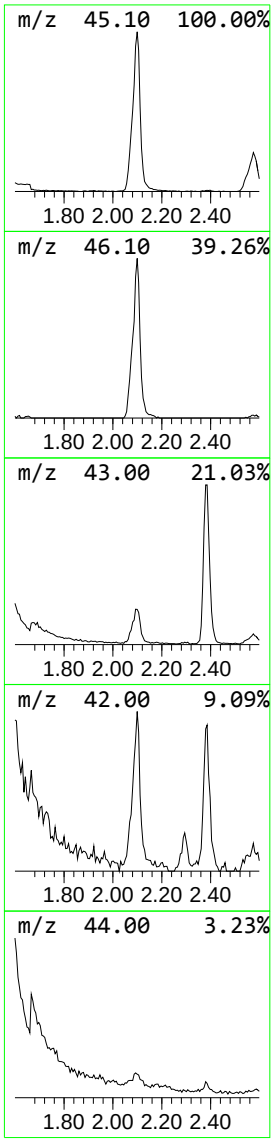
Peak Number 3 Ethanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.099	16.85 ug/l	102993	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	74
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





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Instrument :
MSVOA_X
ClientSampleId :
ORA-1206

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
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TIC Library : C:\Database\NIST20.L
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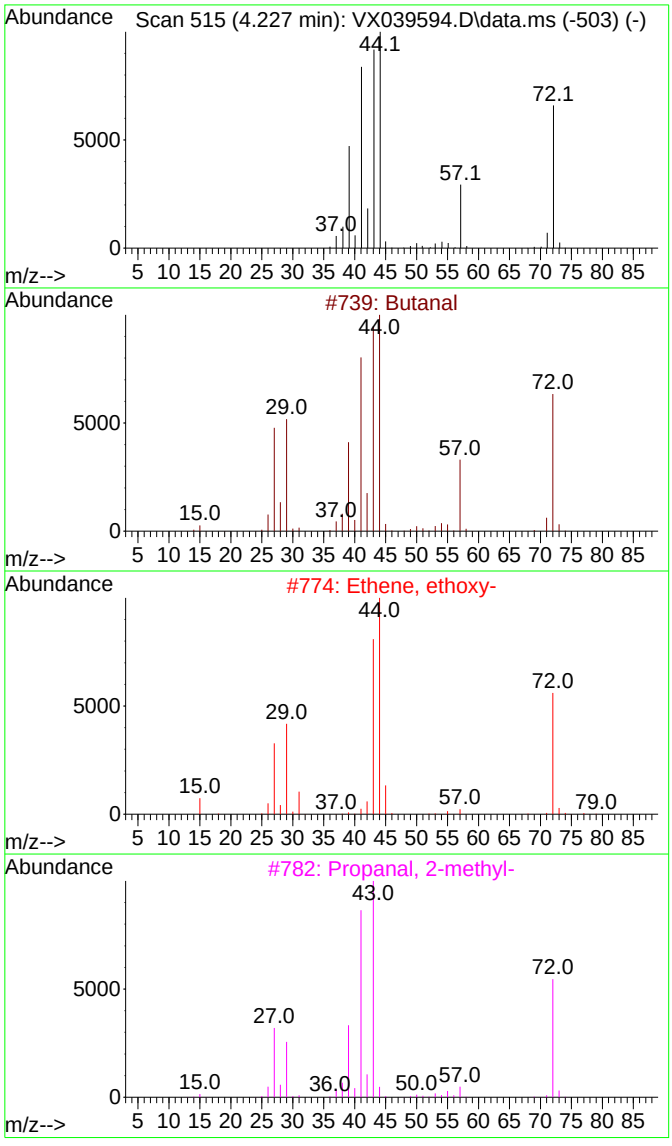
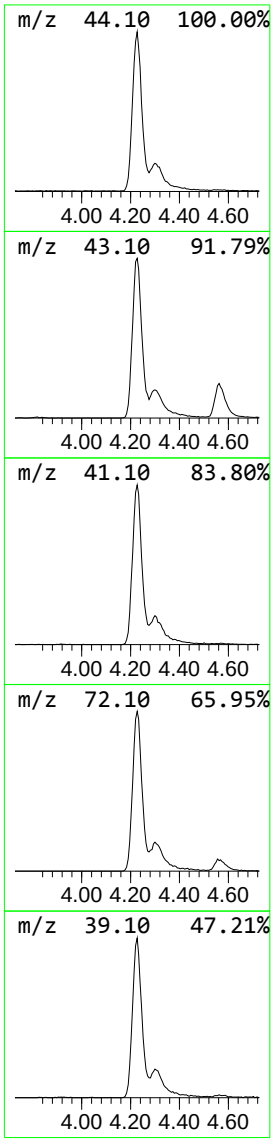
Peak Number 4 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	125.38 ug/l	766419	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	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	32
5	2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	23





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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1206

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

TIC Library : C:\Database\NIST20.L
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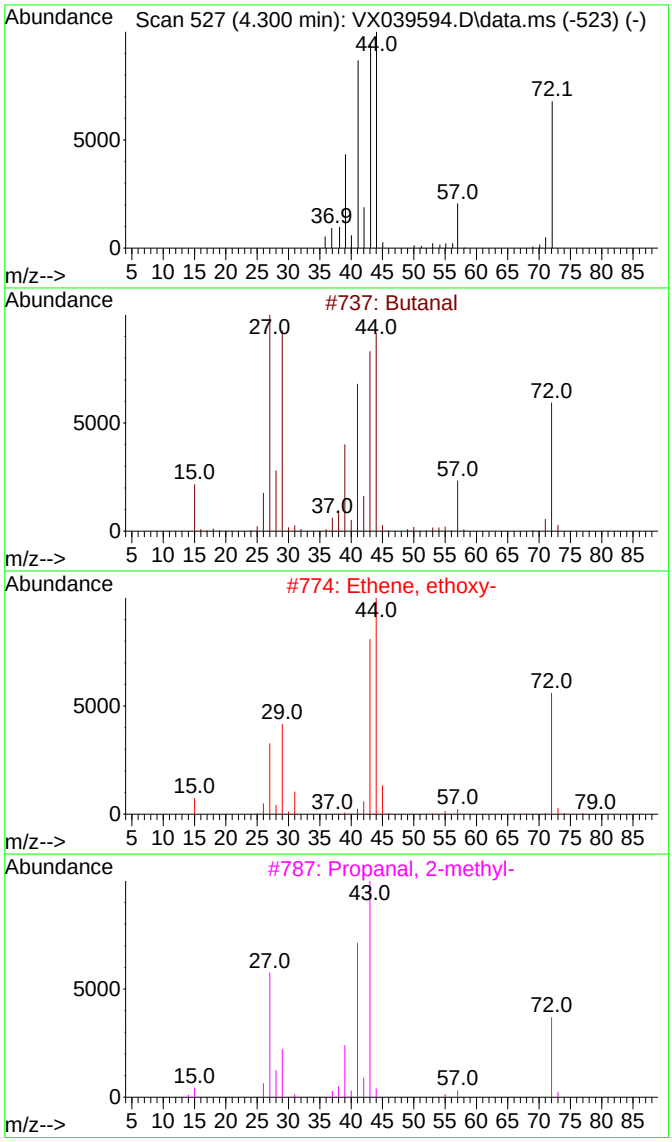
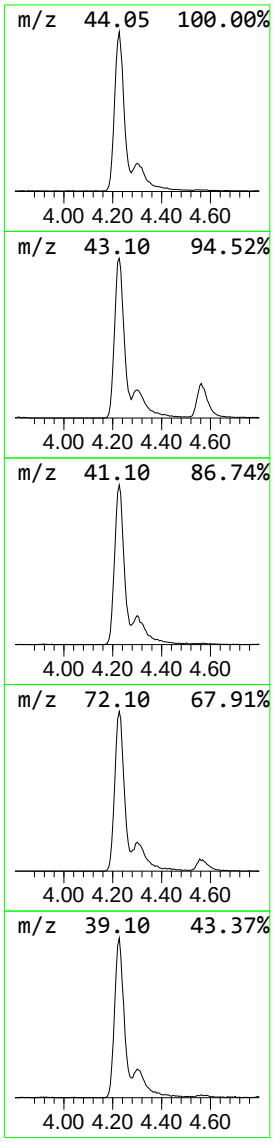
Peak Number 5 unknown4.300 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.300	30.34 ug/l	185450	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	37
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	37
4	Methacrolein	70	C4H6O	000078-85-3	14
5	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	12





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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1206

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

TIC Library : C:\Database\NIST20.L
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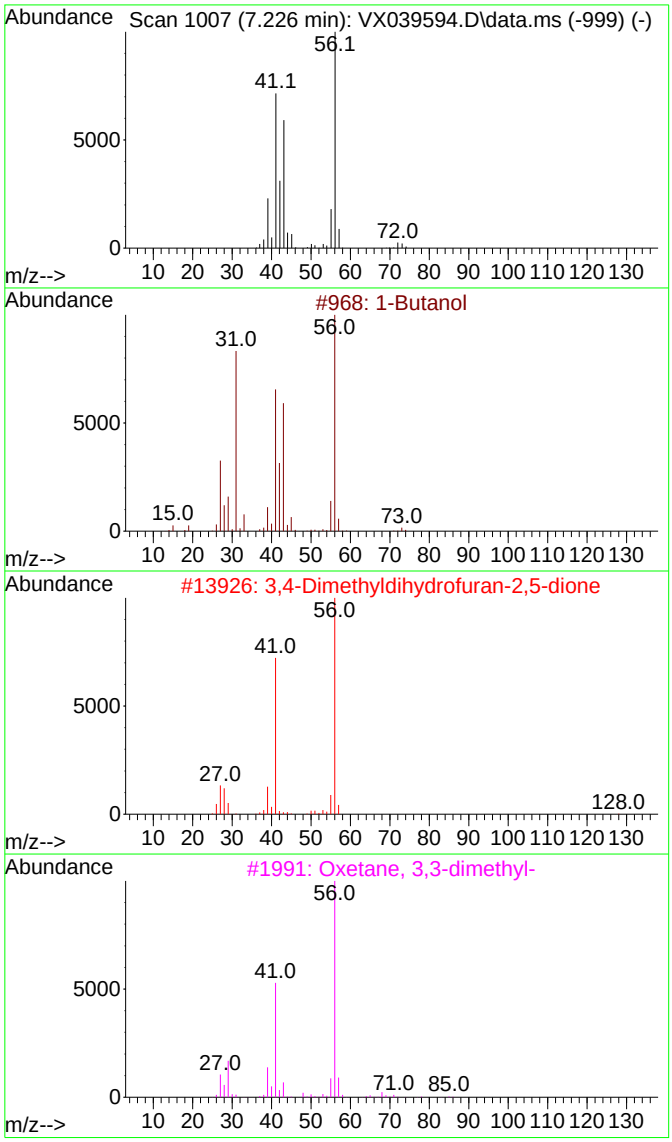
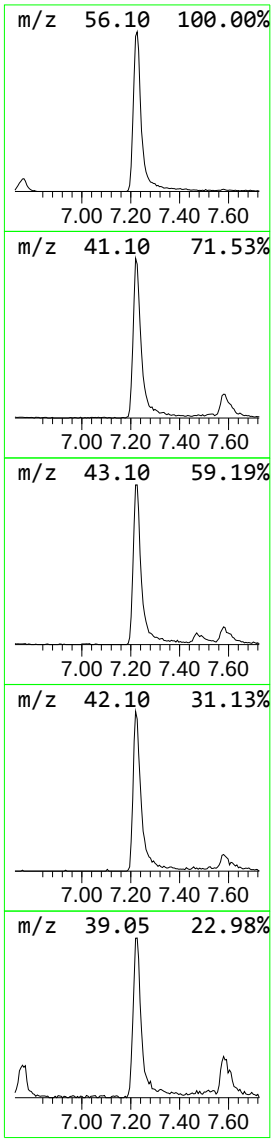
****

Peak Number 6 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.226	26.18 ug/l	255909	1,4-Difluorobenzene	6.757

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	86
2	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	38
3	Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	36
4	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	36
5	Methoxyacetonitrile	71	C3H5NO	001738-36-9	9





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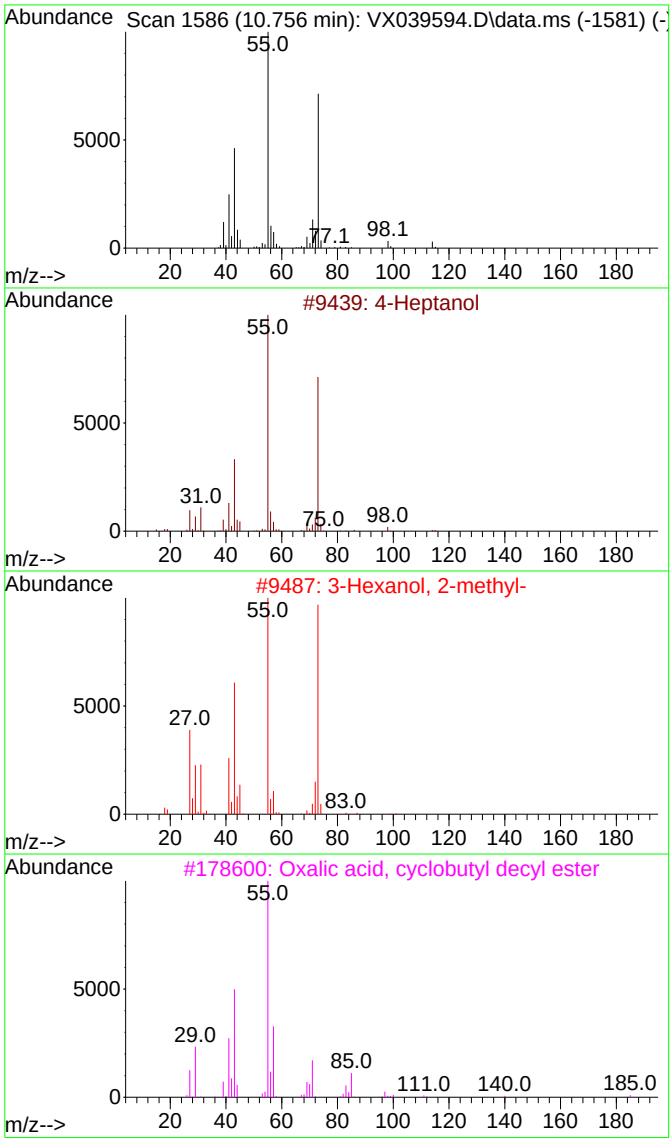
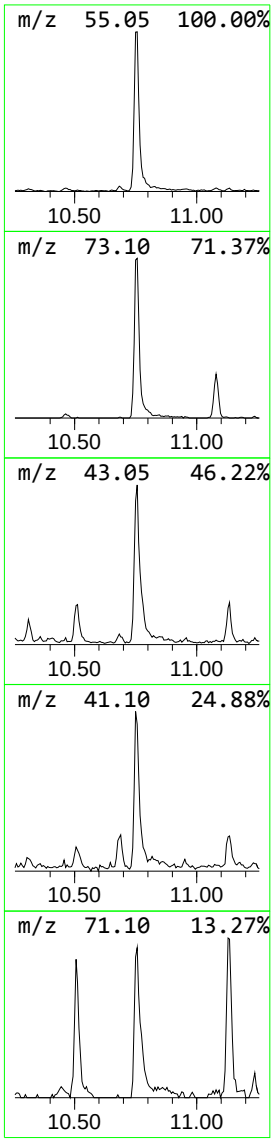
Peak Number 7 4-Heptanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.756	8.97 ug/l	118885	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol	116	C7H16O	000589-55-9	64
2	3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	59
3	Oxalic acid, cyclobutyl decyl ester	284	C16H28O4	1000309-70-1	47
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	43
5	1-Hepten-4-ol	114	C7H14O	003521-91-3	42





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Quant Title : SW846 8260

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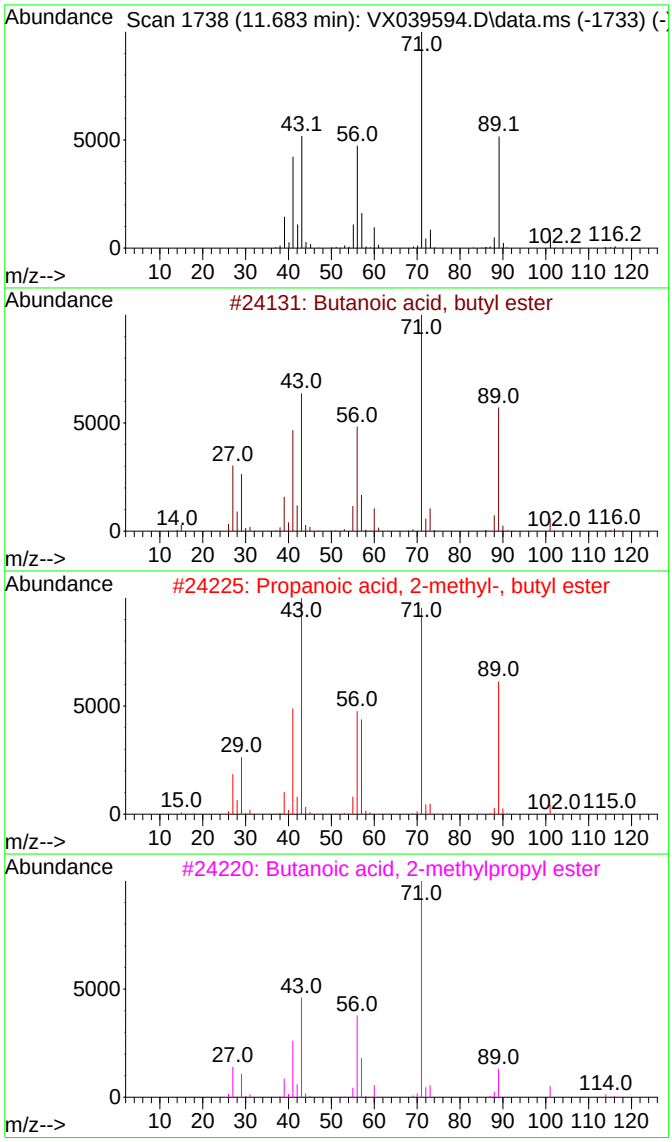
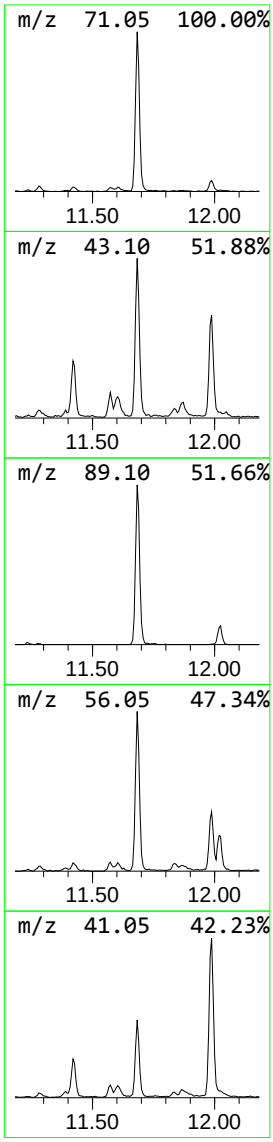
****
Peak Number 8 Butanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.683	17.02 ug/l	198833	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	78
3	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
4	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	72
5	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	64





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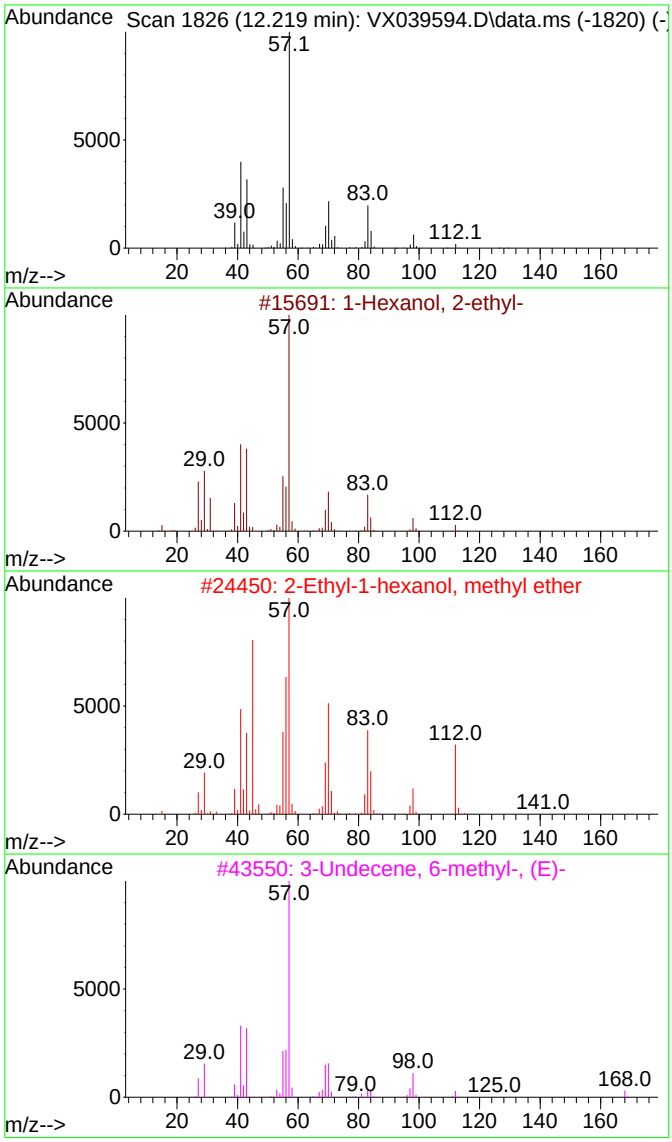
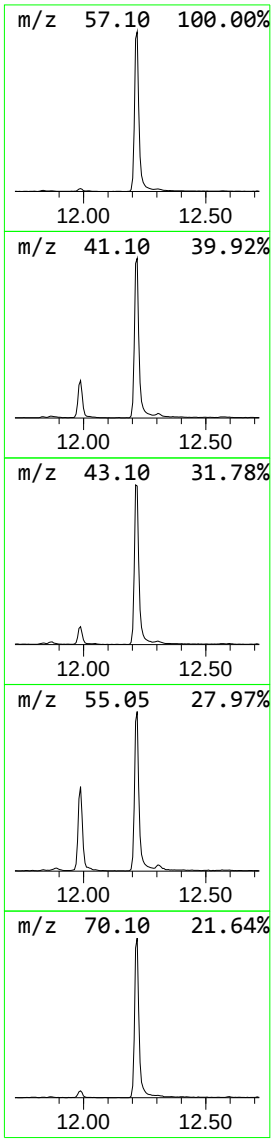
****
Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	157.22 ug/l	1836870	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	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	47
3	3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	47
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5	Carbonic acid, heptyl prop-1-en-...	200	C11H20O3	1000382-54-1	43





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

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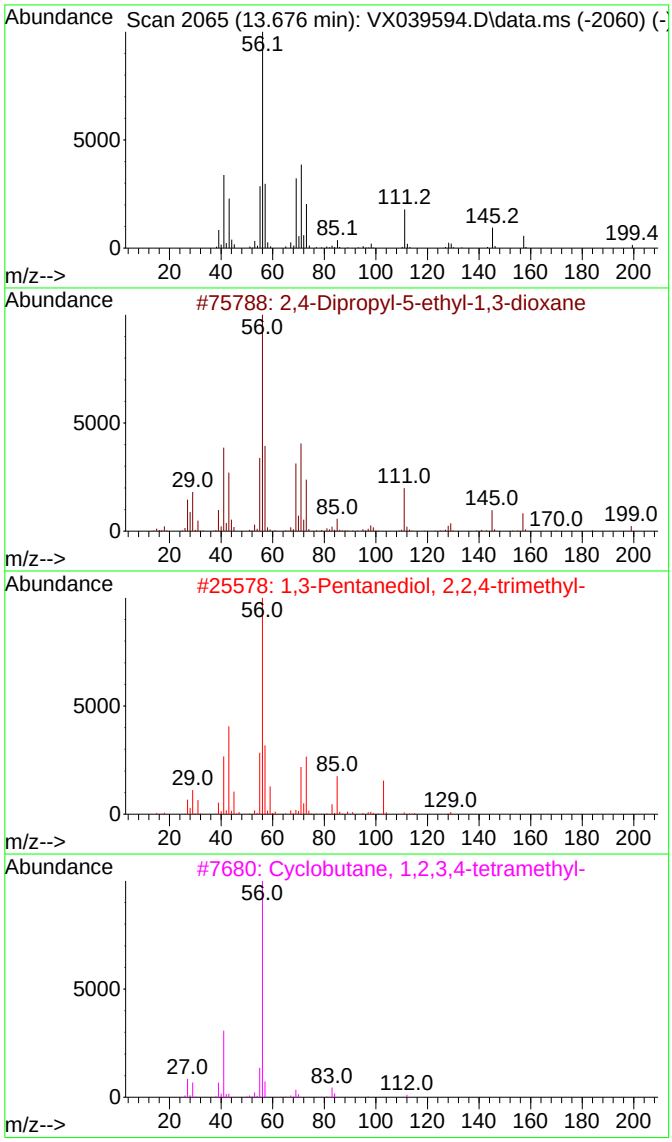
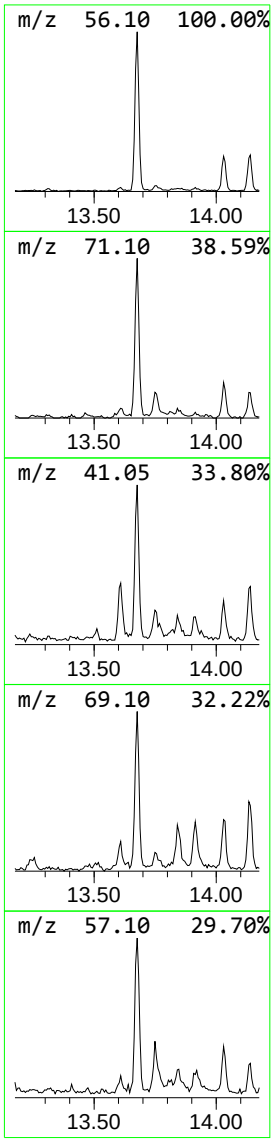
****
Peak Number 10 2,4-Dipropyl-5-ethyl-1,3-di... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.676	9.03 ug/l	105537	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	50
2	1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	28
3	Cyclobutane, 1,2,3,4-tetramethyl-	112	C8H16	069531-57-3	25
4	2-Methyl-1-nonene	140	C10H20	002980-71-4	25
5	Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	23





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010324\
Data File : VX039594.D
Acq On : 03 Jan 2024 12:12
Operator : JC/MD
Sample : P1001-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
ORA-1206

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	1.514	95.5	ug/l	583641	1	5.550	305628	50.0
Ethanol	2.099	16.9	ug/l	102993	1	5.550	305628	50.0
Butanal	4.227	125.4	ug/l	766419	1	5.550	305628	50.0
unknown4.300	4.300	30.3	ug/l	185450	1	5.550	305628	50.0
1-Butanol	7.226	26.2	ug/l	255909	2	6.757	488734	50.0
4-Heptanol	10.756	9.0	ug/l	118885	3	10.055	662617	50.0
Butanoic acid, ...	11.683	17.0	ug/l	198833	4	12.024	584159	50.0
1-Hexanol, 2-et...	12.219	157.2	ug/l	1836870	4	12.024	584159	50.0
2,4-Dipropyl-5-...	13.676	9.0	ug/l	105537	4	12.024	584159	50.0