LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX061323\
Data File : VX036150.D
Acq On : 13 Jun 2023 17:36
Operator : JC/MD
Sample : 03170-02 100X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-2012

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\82X053123W.M
Title : SW846 8260

Signal : TIC: VX036150.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	16	rVB	11794	12733	1.18%	0.170%
2	1.459	56	61	74	rBV	304868	460250	42.68%	6.157%
3	2.398	209	215	225	rVB	5441	12842	1.19%	0.172%
4	2.617	237	251	252	rBV3	7418	19306	1.79%	0.258%
5	3.324	357	367	381	rBV	29379	68054	6.31%	0.910%
6	4.397	532	543	556	rBV	25614	92401	8.57%	1.236%
7	4.568	564	571	573	rBV3	5740	10789	1.00%	0.144%
8	5.385	692	705	717	rBV	118564	344706	31.96%	4.611%
9	5.550	721	732	748	rVB	236738	665718	61.73%	8.905%
10	5.958	788	799	811	rBV	149047	402919	37.36%	5.390%
11	6.354	854	864	879	rBV3	32326	91593	8.49%	1.225%
12	6.598	896	904	914	rBV2	23946	61356	5.69%	0.821%
13	6.763	920	931	942	rBV	346390	830415	77.00%	11.108%
14	6.879	942	950	961	rVB	49189	120088	11.14%	1.606%
15	7.214	996	1005	1014	rBV3	7927	19086	1.77%	0.255%
16	8.647	1233	1240	1249	rBV	708623	1078441	100.00%	14.426%
17	9.872	1436	1441	1448	rBV5	13127	32673	3.03%	0.437%
18	10.055	1465	1471	1481	rBV	711507	959301	88.95%	12.832%
19	10.939	1610	1616	1633	rBV	79315	171365	15.89%	2.292%
20	11.079	1633	1639	1646	rVV	610308	753702	69.89%	10.082%
21	11.146	1646	1650	1656	rVB2	8141	11523	1.07%	0.154%
22	11.878	1766	1770	1781	rVB	22488	38498	3.57%	0.515%
23	12.018	1788	1793	1802	rVB	732965	924427	85.72%	12.366%
24	12.219	1820	1826	1834	rBV2	30353	51104	4.74%	0.684%
25	12.554	1876	1881	1886	rBV	31160	51242	4.75%	0.685%
26	13.207	1983	1988	1993	rBV	8604	12339	1.14%	0.165%
27	13.591	2045	2051	2060	rBV7	5600	11465	1.06%	0.153%
28	13.725	2069	2073	2077	rBV3	10665	16124	1.50%	0.216%
29	13.774	2077	2081	2087	rVB	71907	89815	8.33%	1.201%
30	14.438	2186	2190	2199	rBV	6816	13481	1.25%	0.180%
31	14.633	2214	2222	2228	rVB	19964	29178	2.71%	0.390%
32	14.780	2240	2246	2252	rVB	14968	18739	1.74%	0.251%

Sum of corrected areas: 7475673

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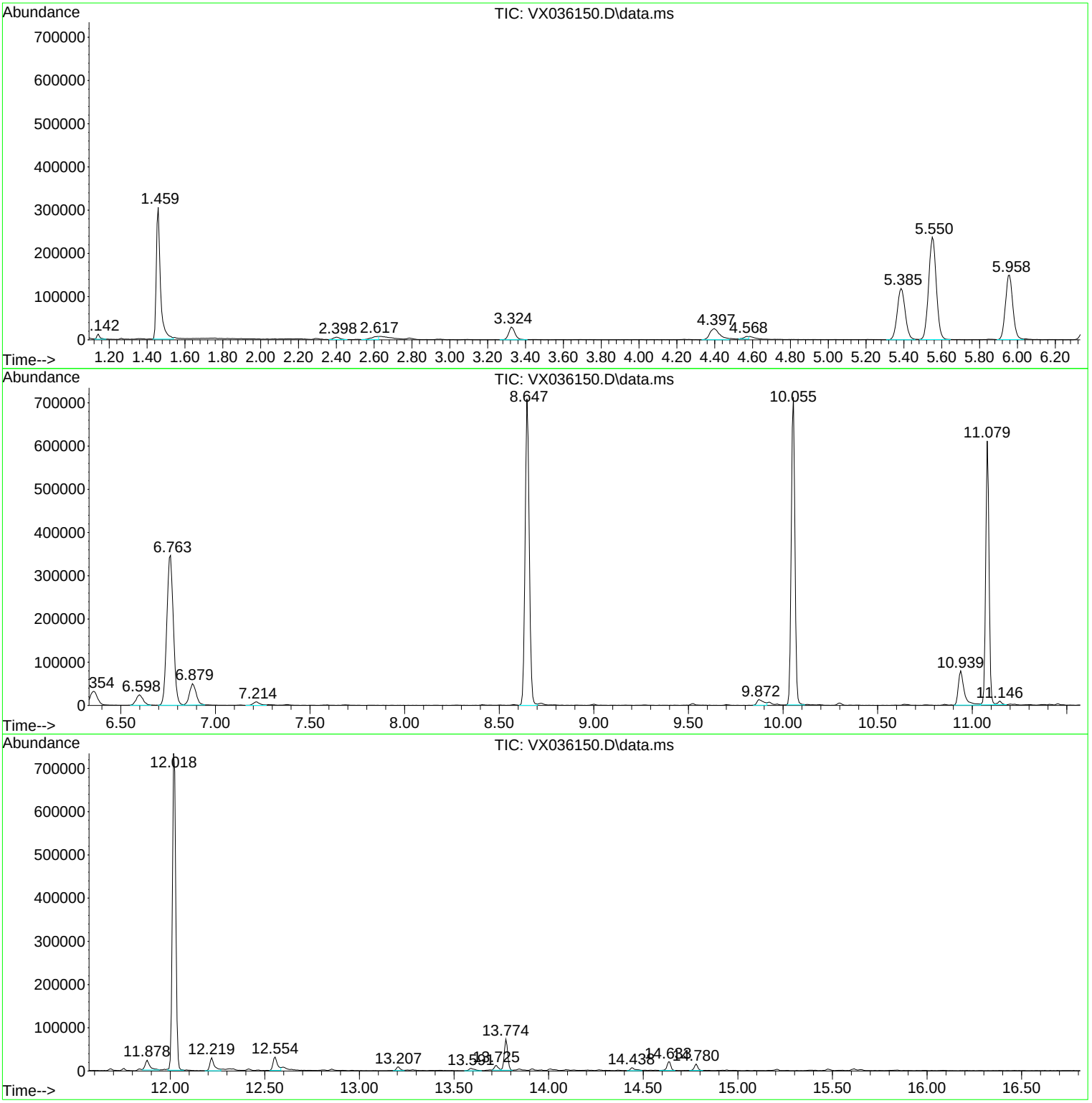
Instrument :
MSVOA_X
ClientSampleId :
AUD-2012

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053123W.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

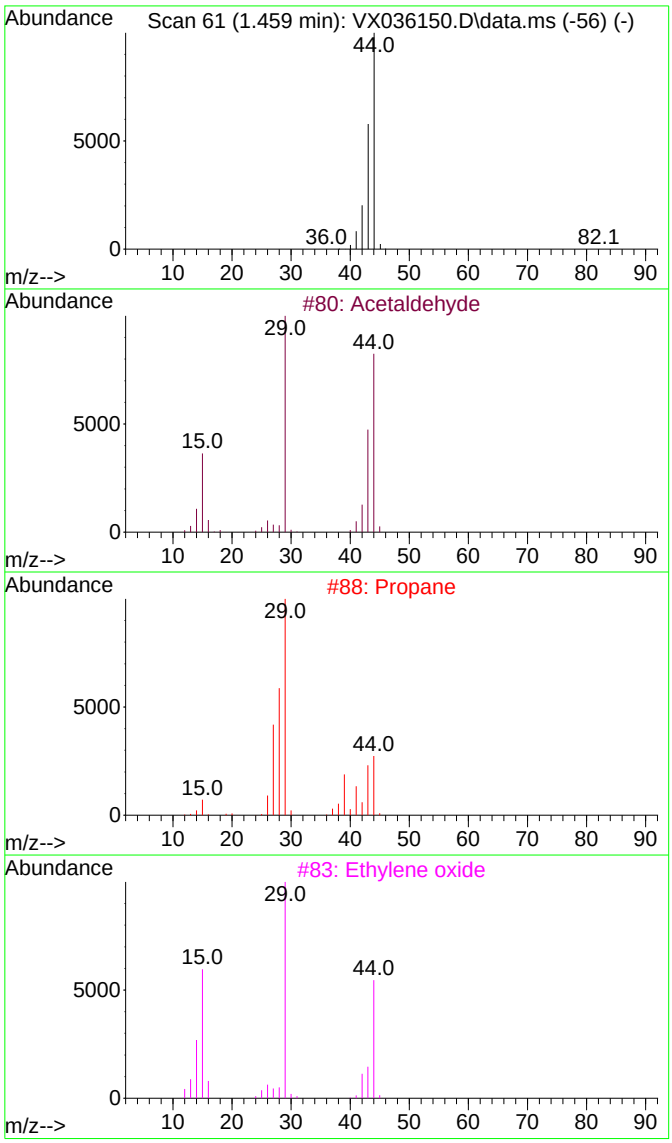
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

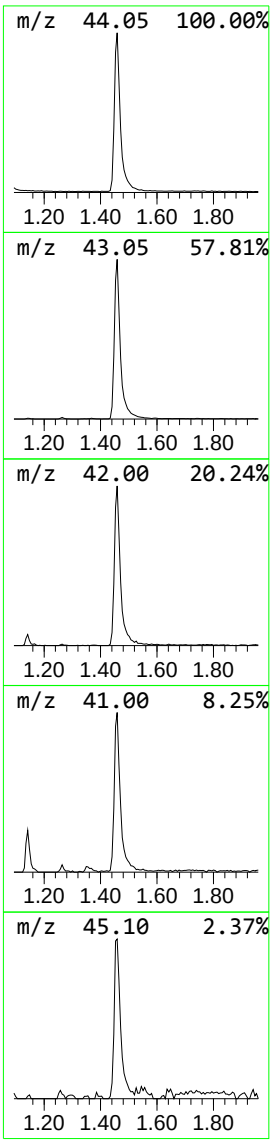
****

Peak Number 1 unknown1.459 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.459	34.57 ug/l	460250	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	9
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Hydrogen isocyanate	43	CHNO	000075-13-8	3
5	Carbon dioxide	44	CO2	000124-38-9	3





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Data File : VX036150.D
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Instrument :
MSVOA_X
ClientSampleId :
AUD-2012

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053123W.M
Quant Title : SW846 8260

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

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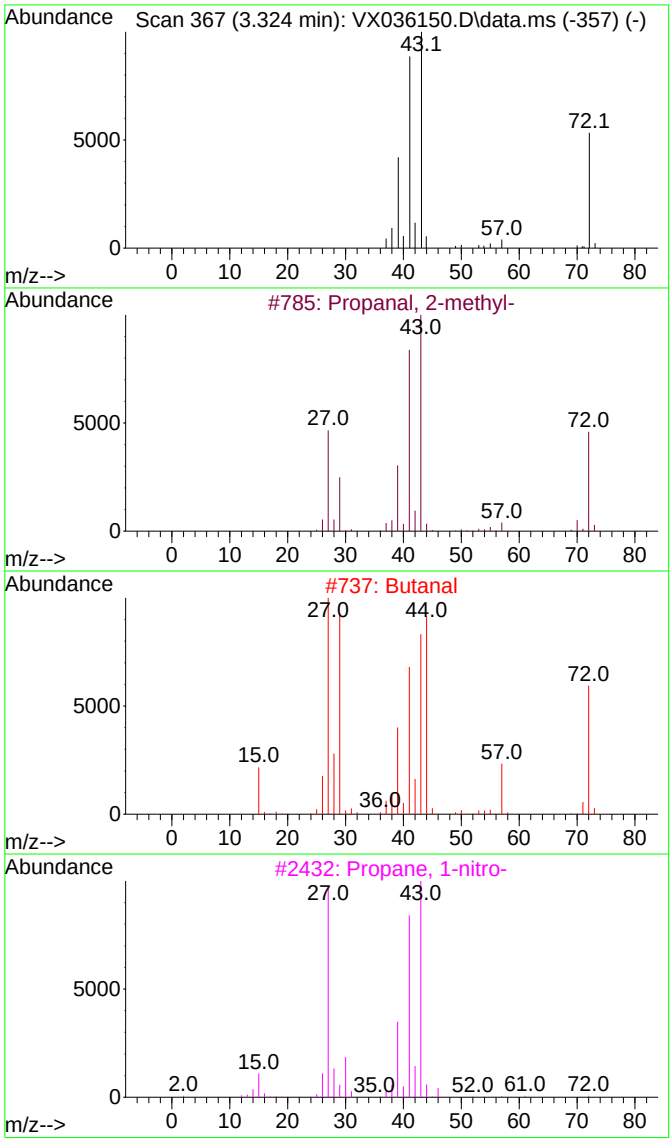
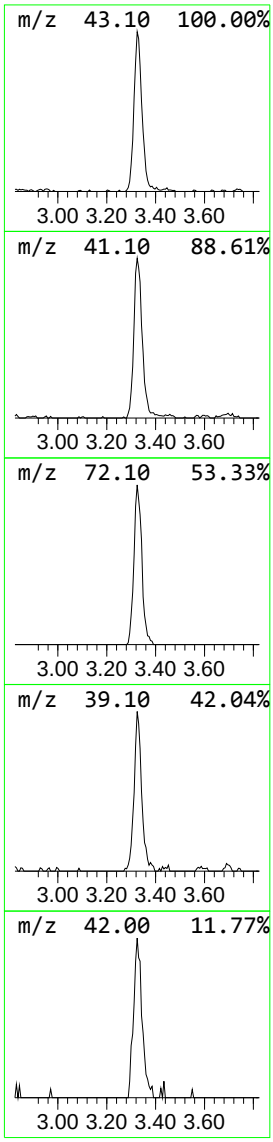
Peak Number 2 Propanal, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.324	5.11 ug/l	68054	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal, 2-methyl-	72	C4H8O	000078-84-2	91
2	Butanal	72	C4H8O	000123-72-8	64
3	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	40
4	Methacrolein	70	C4H6O	000078-85-3	35
5	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	33





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Instrument :
MSVOA_X
ClientSampleId :
AUD-2012

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053123W.M
Quant Title : SW846 8260

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

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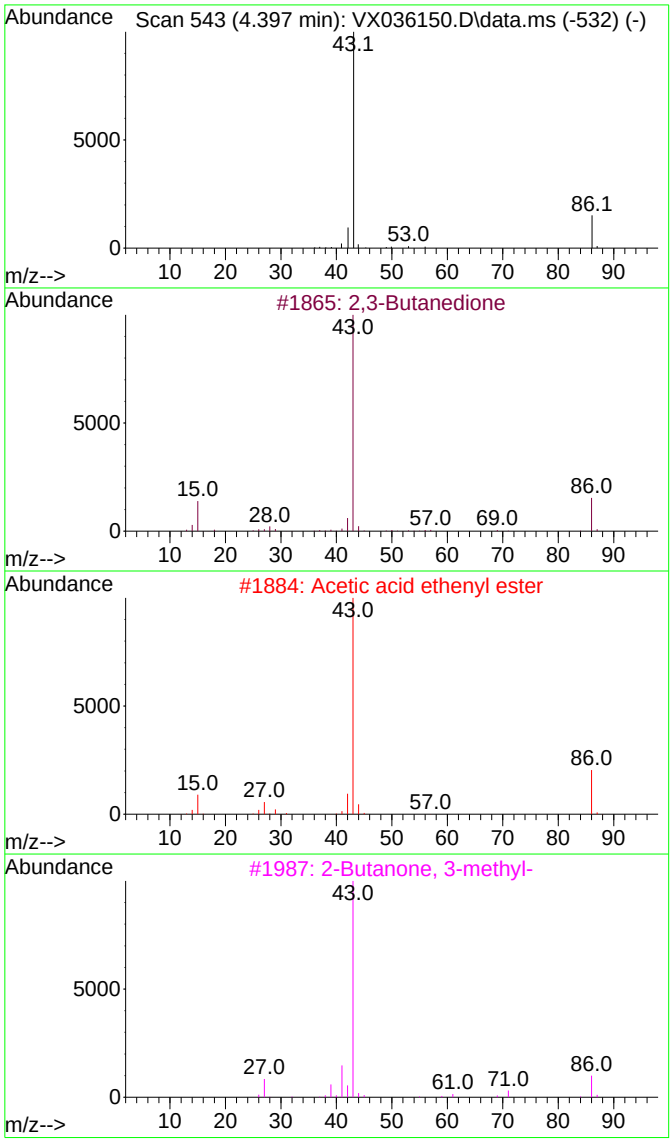
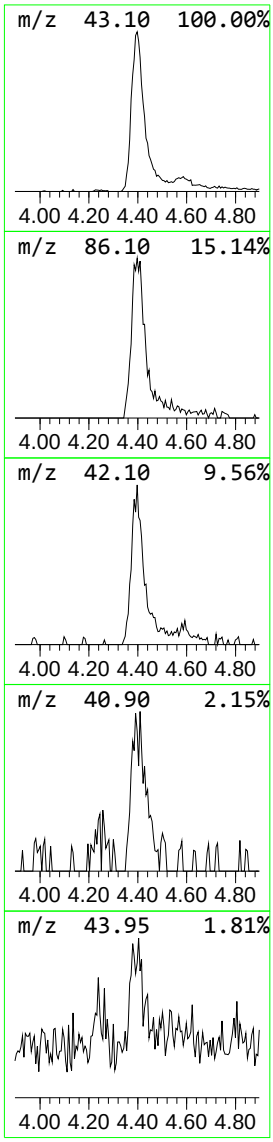
Peak Number 3 2,3-Butanedione Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.397	6.94 ug/l	92401	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione	86	C4H6O2	000431-03-8	72
2	Acetic acid ethenyl ester	86	C4H6O2	000108-05-4	9
3	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9
4	2-Pentanone	86	C5H10O	000107-87-9	7
5	Ethanone, 1-oxiranyl-	86	C4H6O2	004401-11-0	7





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Instrument :
MSVOA_X
ClientSampleId :
AUD-2012

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053123W.M
Quant Title : SW846 8260

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

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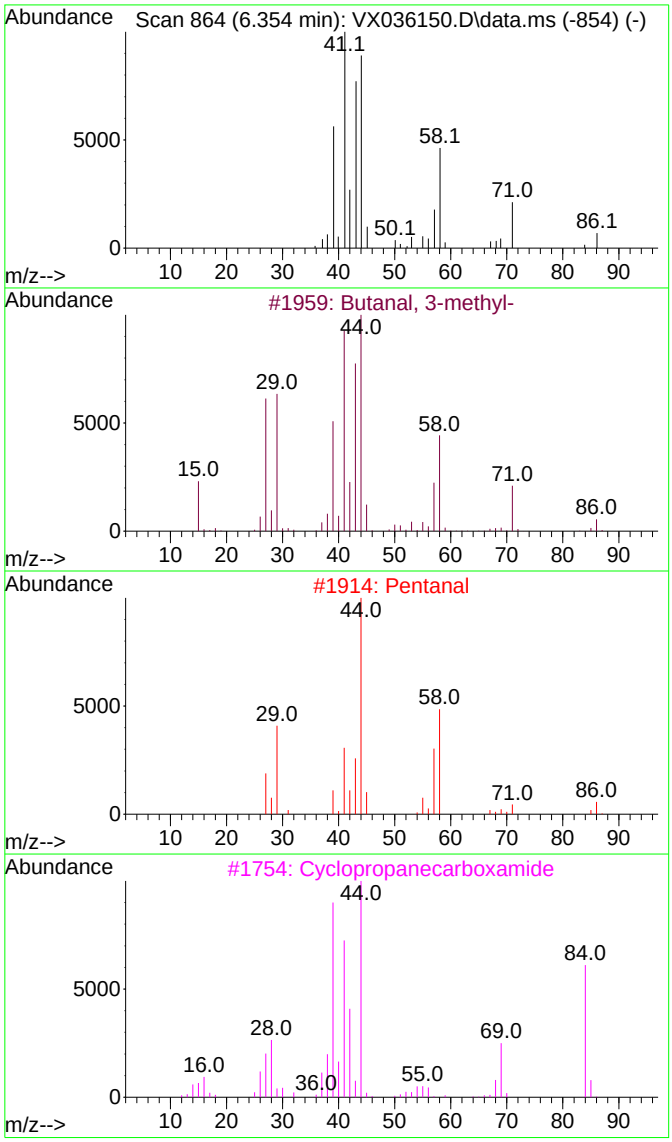
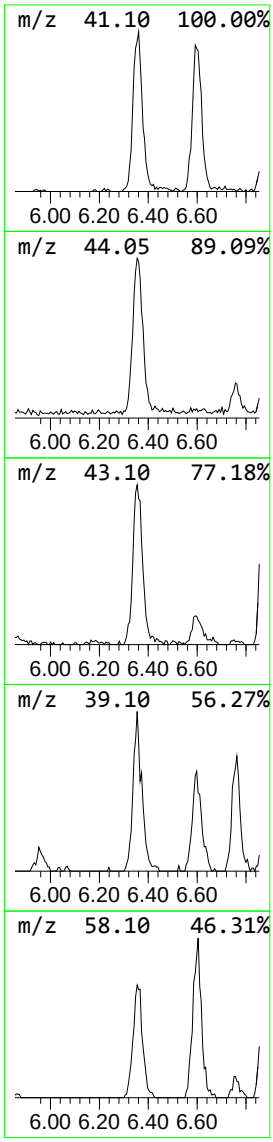
Peak Number 4 Butanal, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.354	5.51 ug/l	91593	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal, 3-methyl-	86	C5H10O	000590-86-3	95
2	Pentanal	86	C5H10O	000110-62-3	43
3	Cyclopropanecarboxamide	85	C4H7NO	006228-73-5	20
4	2H-Pyran-2-one, tetrahydro-6,6-d...	128	C7H12O2	002610-95-9	10
5	Cyclopropanecarboxylic acid	86	C4H6O2	001759-53-1	9





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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
AUD-2012

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X053123W.M
Quant Title : SW846 8260

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

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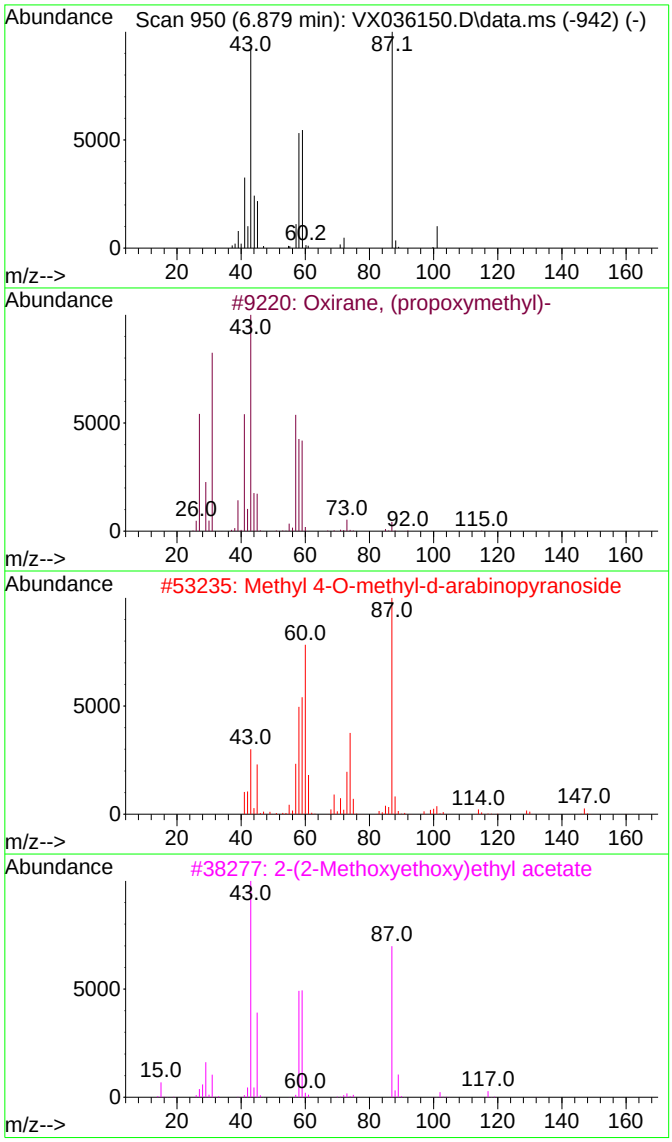
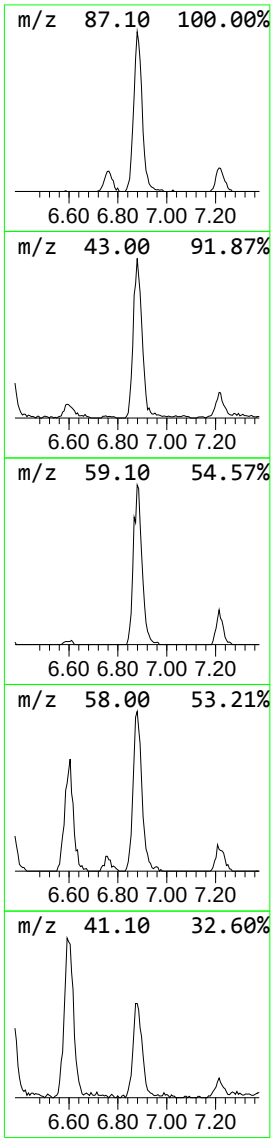
Peak Number 5 unknown6.879 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.879	7.23 ug/l	120088	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, (propoxymethyl)-	116	C6H12O2	003126-95-2	37
2	Methyl 4-O-methyl-d-arabinopyran...	178	C7H14O5	1000129-79-9	36
3	2-(2-Methoxyethoxy)ethyl acetate	162	C7H14O4	1000351-95-4	36
4	1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	36
5	Monomethyl malonate	118	C4H6O4	016695-14-0	28





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AUD-2012

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Quant Title : SW846 8260

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

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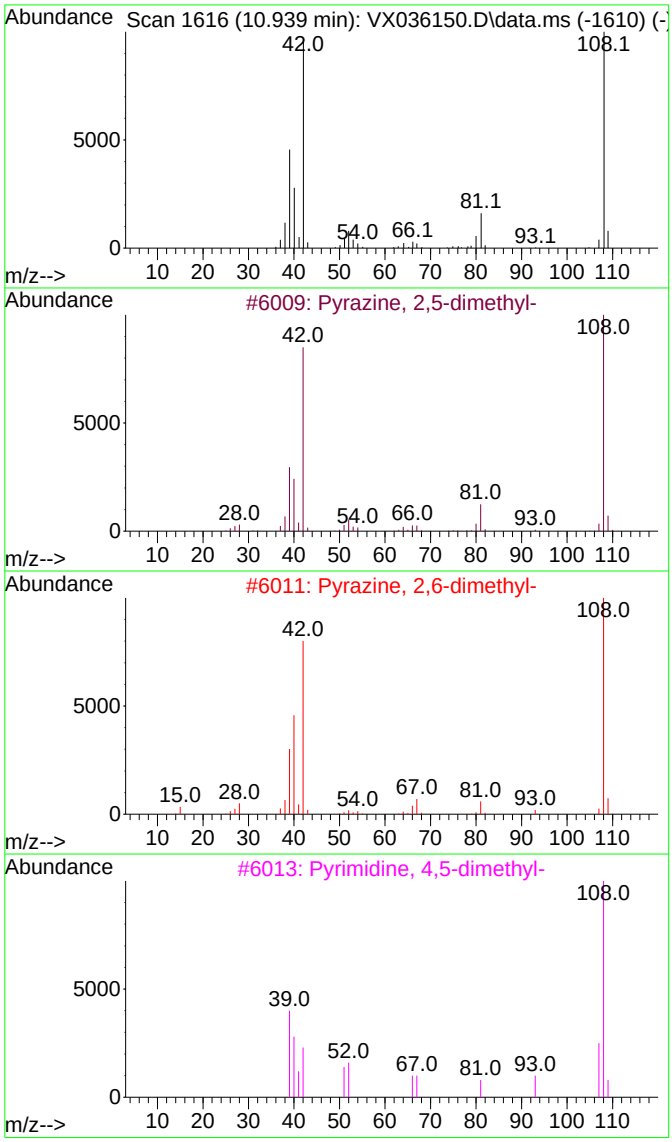
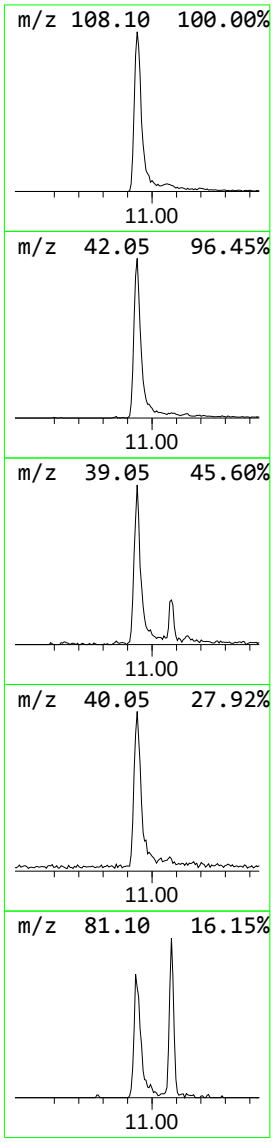
Peak Number 6 Pyrazine, 2,5-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.939	8.93 ug/l	171365	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrazine, 2,5-dimethyl-	108	C6H8N2	000123-32-0	94
2	Pyrazine, 2,6-dimethyl-	108	C6H8N2	000108-50-9	64
3	Pyrimidine, 4,5-dimethyl-	108	C6H8N2	000694-81-5	50
4	Cyclopropane	42	C3H6	000075-19-4	43
5	(4H-[1,2,4]Triazol-3-yl)acetonit...	108	C4H4N4	1000304-53-5	42





Tentatively Identified Compound (LSC) summary

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown1.459	1.459	34.6	ug/l	460250	1	5.550	665718	50.0
Propanal, 2-met...	3.324	5.1	ug/l	68054	1	5.550	665718	50.0
2,3-Butanedione	4.397	6.9	ug/l	92401	1	5.550	665718	50.0
Butanal, 3-methyl-	6.354	5.5	ug/l	91593	2	6.763	830415	50.0
unknown6.879	6.879	7.2	ug/l	120088	2	6.763	830415	50.0
Pyrazine, 2,5-d...	10.939	8.9	ug/l	171365	3	10.055	959301	50.0