LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032421\
Data File : VX021437.D
Acq On : 24 Mar 2021 15:50
Operator : JC/MD
Sample : M1752-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : COMP2-41720:23-41718

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\82X032421W.M
Title : SW846 8260

Signal : TIC: VX021437.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.470	61	65	79	rBV	8765377	10474347	100.00%	61.969%
2	2.099	166	172	183	rBV	105639	160093	1.53%	0.947%
3	5.464	731	744	757	rBV	52273	152030	1.45%	0.899%
4	5.635	762	773	786	rVB	79328	220944	2.11%	1.307%
5	6.035	831	841	847	rBV	55967	144024	1.38%	0.852%
6	6.111	847	854	865	rVB	97197	254621	2.43%	1.506%
7	6.829	966	976	988	rBV	128899	305928	2.92%	1.810%
8	8.694	1286	1293	1300	rBV	265650	426191	4.07%	2.521%
9	8.765	1300	1305	1311	rVB	225279	334552	3.19%	1.979%
10	9.530	1431	1435	1447	rVB	309127	469071	4.48%	2.775%
11	10.094	1524	1531	1535	rBV	287193	410444	3.92%	2.428%
12	10.136	1535	1538	1543	rVB	117954	154356	1.47%	0.913%
13	10.347	1565	1574	1585	rVB3	360314	585279	5.59%	3.463%
14	10.447	1585	1591	1604	rBV2	64629	105010	1.00%	0.621%
15	10.683	1626	1631	1640	rVB2	194920	295060	2.82%	1.746%
16	11.118	1699	1705	1711	rBV	243358	324468	3.10%	1.920%
17	11.724	1804	1808	1815	rVV2	70348	119852	1.14%	0.709%
18	11.789	1815	1819	1824	rVB	95329	117242	1.12%	0.694%
19	12.059	1861	1865	1872	rVB	290492	358709	3.42%	2.122%
20	12.253	1888	1898	1909	rBV	292848	448623	4.28%	2.654%
21	12.453	1926	1932	1938	rVB	166746	210017	2.01%	1.243%
22	13.818	2156	2164	2170	rBV	567273	721299	6.89%	4.267%
23	14.677	2305	2310	2317	rVB	94961	110373	1.05%	0.653%

Sum of corrected areas: 16902533

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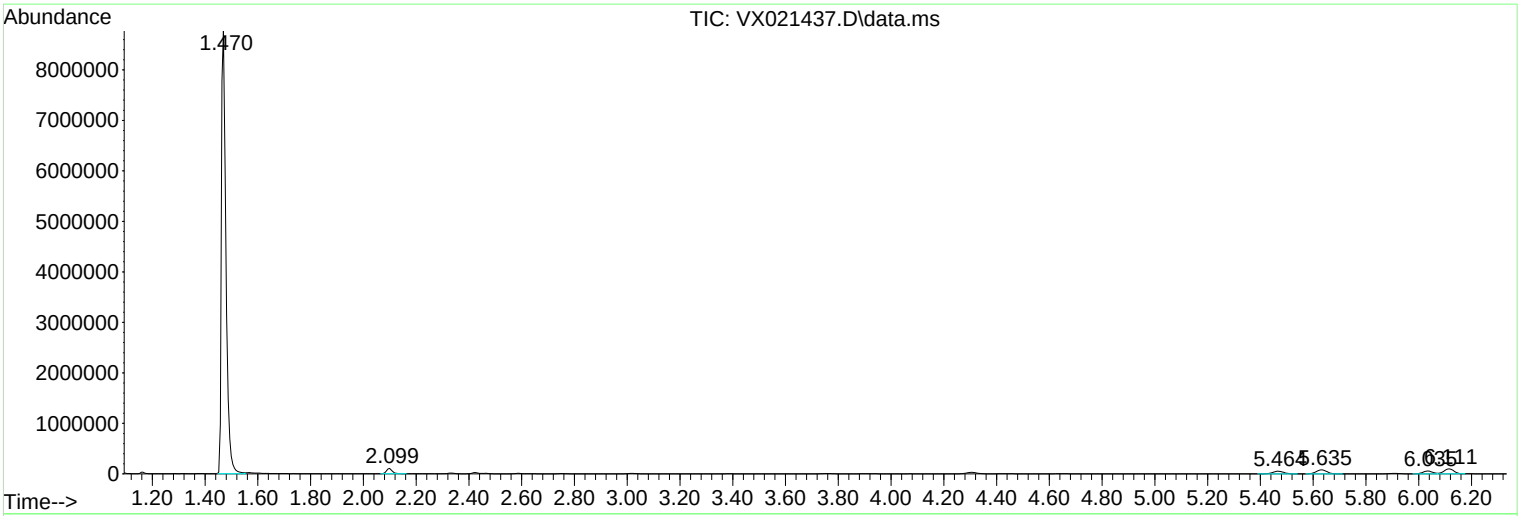
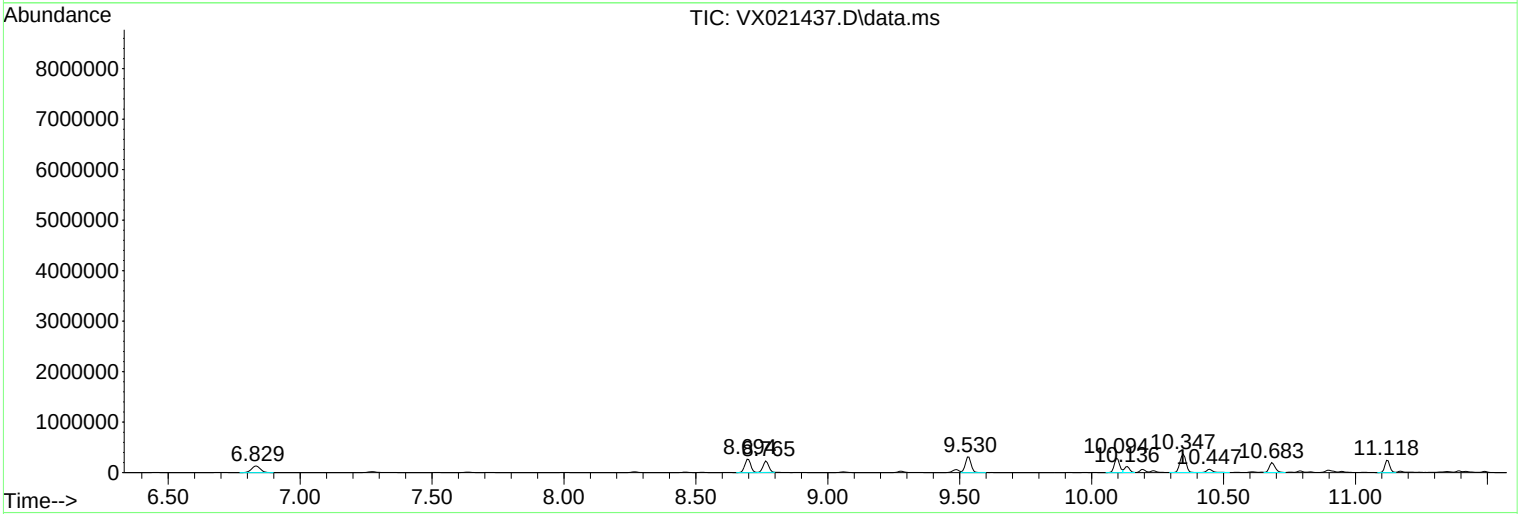
ALS Vial : 16 Sample Multiplier: 1

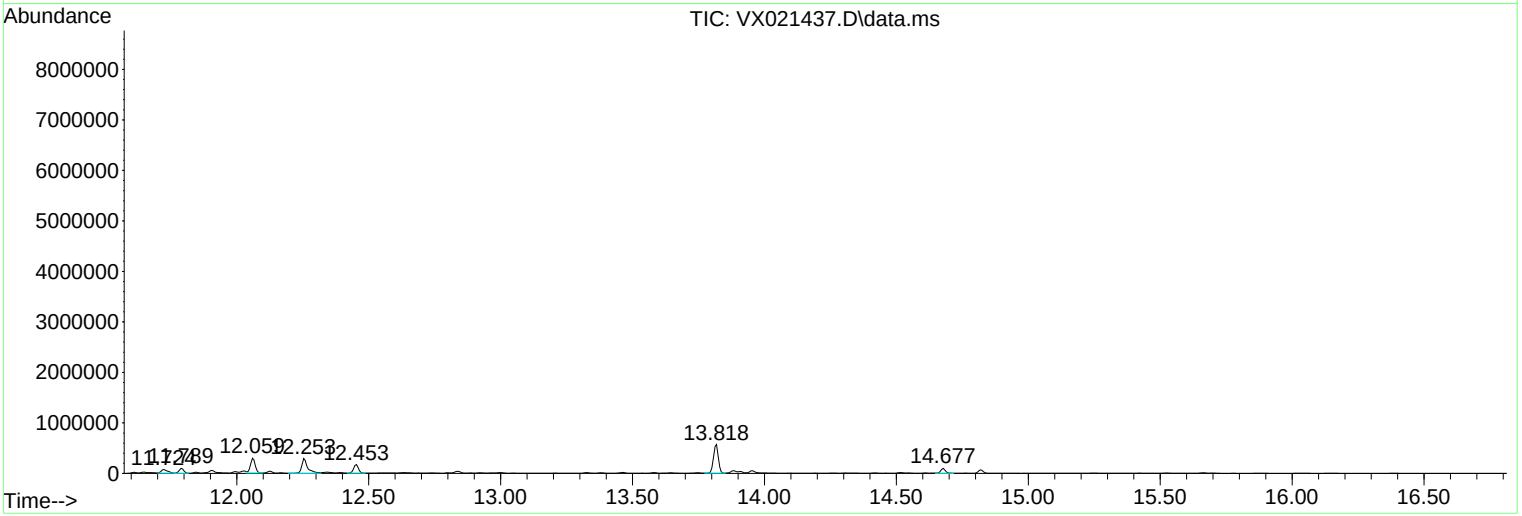
Instrument :
MSVOA_X
ClientSampleId :
COMP2-41720:23-41718

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P







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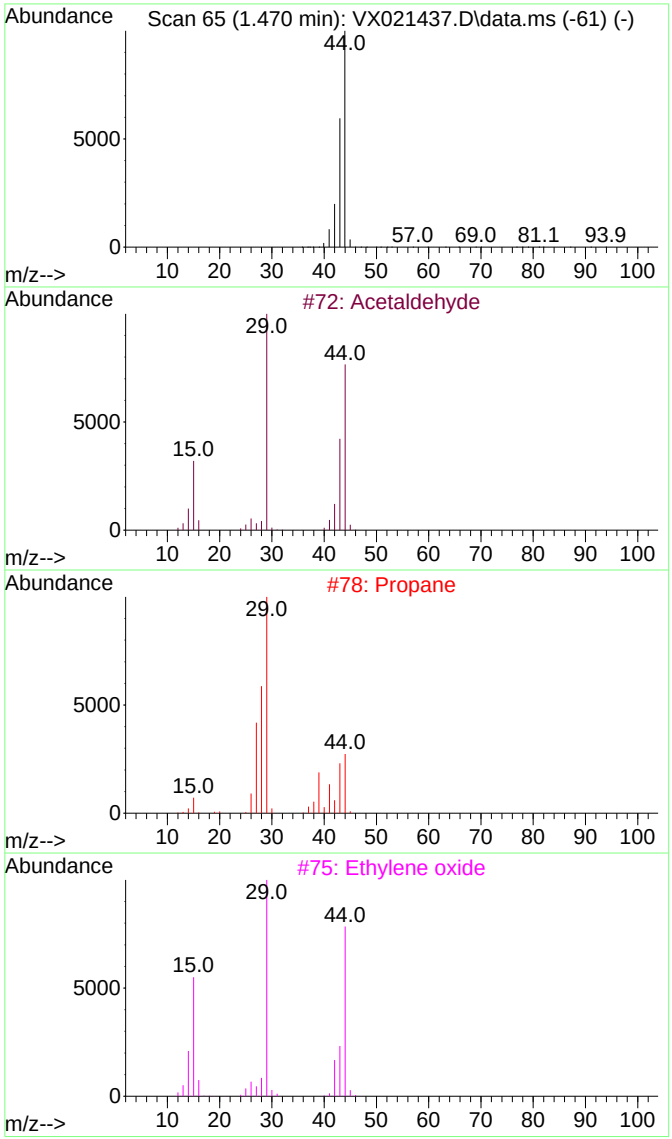
Quant Title : SW846 8260

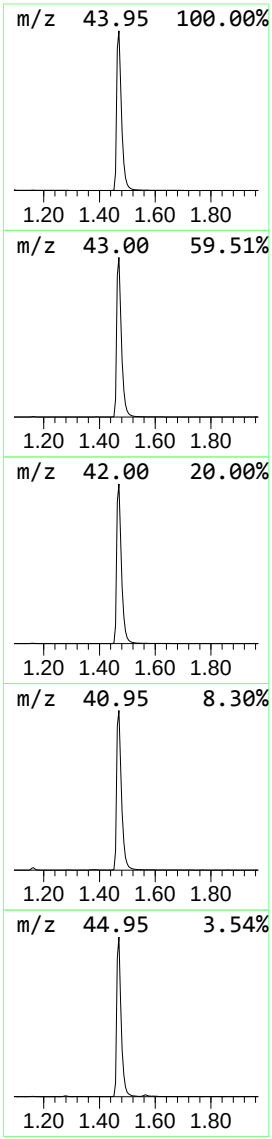
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.470	2370.36 ug/l	10474300	Pentafluorobenzene	5.635

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	Ethyne, fluoro-	44	C2HF	002713-09-9	3





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Data File : VX021437.D
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Operator : JC/MD
Sample : M1752-07
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP2-41720:23-41718

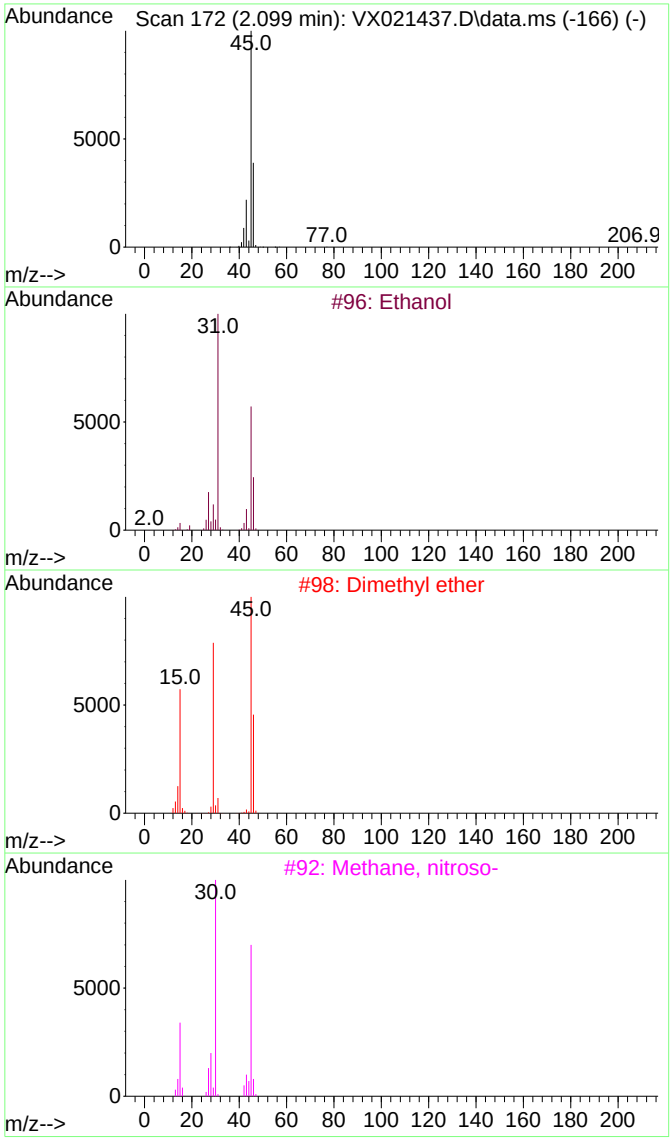
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

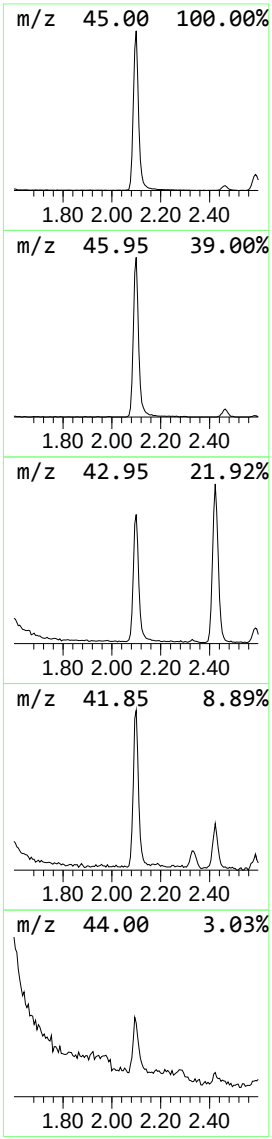
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.099	36.23 ug/l	160093	Pentafluorobenzene	5.635

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





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP2-41720:23-41718

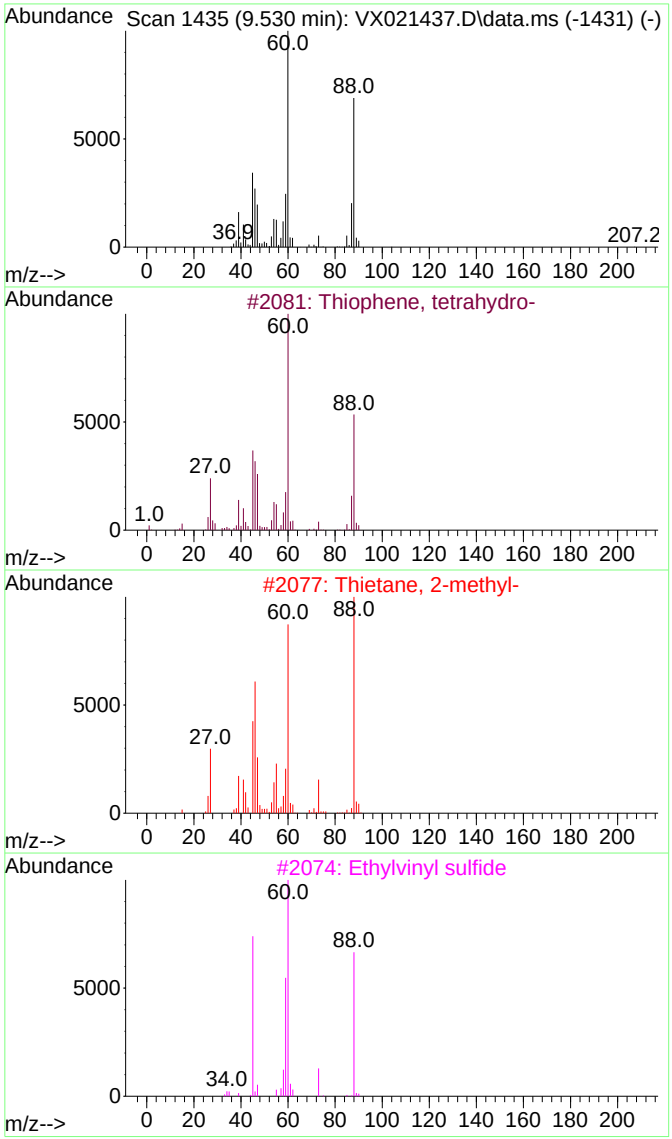
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

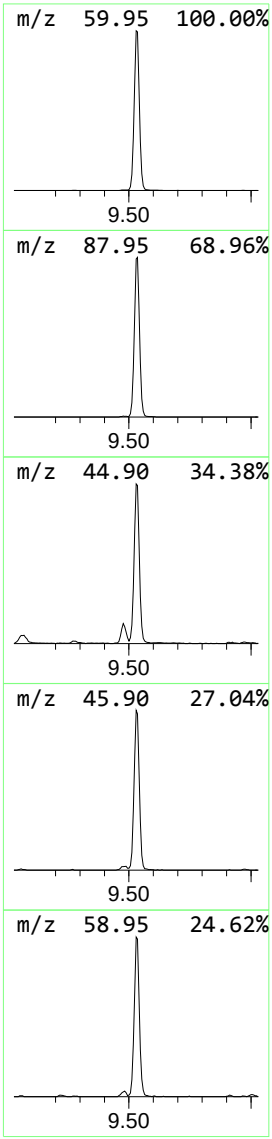
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Thiophene, tetrahydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.530	57.14 ug/l	469071	Chlorobenzene-d5	10.094

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-	88	C4H8S	000110-01-0	93
2	Thietane, 2-methyl-	88	C4H8S	017837-41-1	72
3	Ethylvinyl sulfide	88	C4H8S	000627-50-9	38
4	1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	33
5	4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	23





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Operator : JC/MD
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP2-41720:23-41718

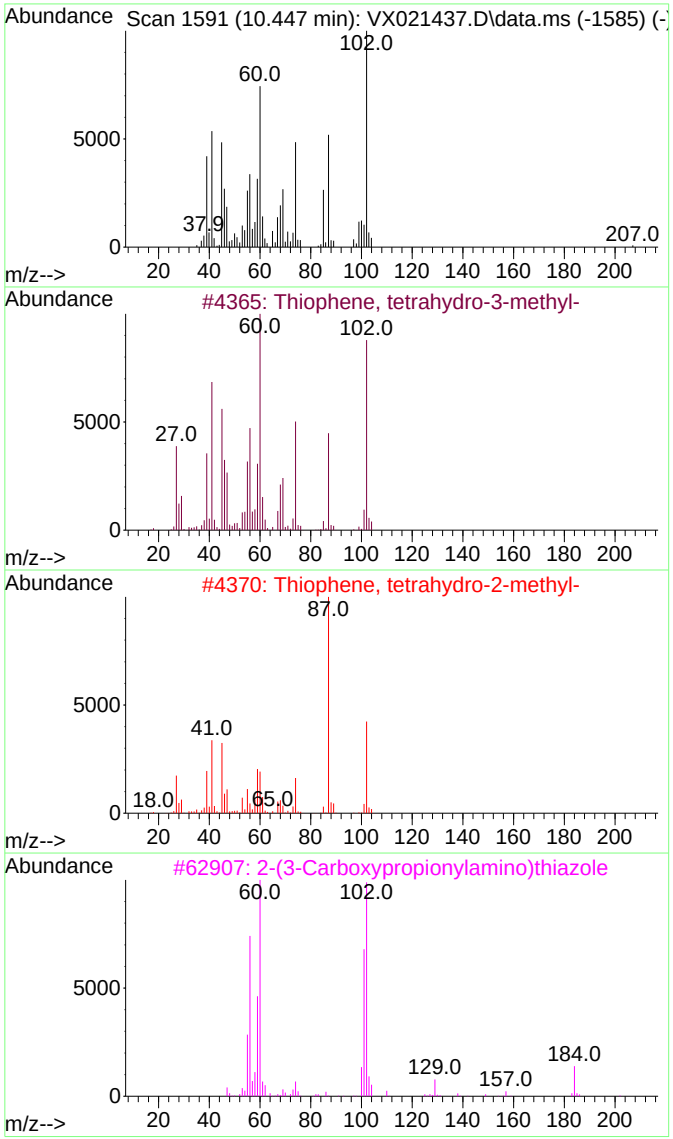
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

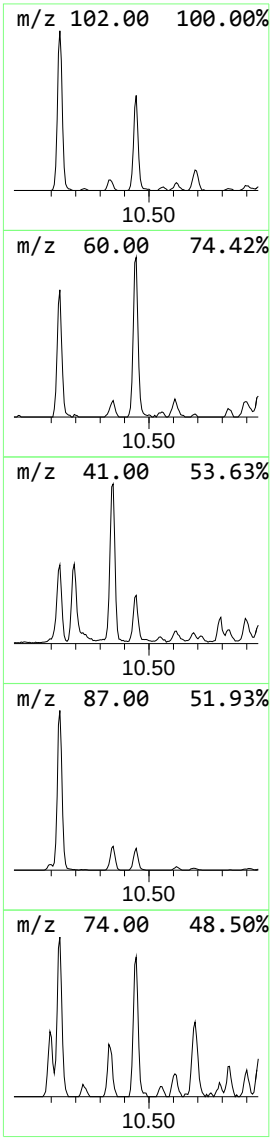
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Thiophene, tetrahydro-3-met... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.447	12.79 ug/l	105010	Chlorobenzene-d5	10.094

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiophene, tetrahydro-3-methyl-	102	C5H10S	004740-00-5	95
2	Thiophene, tetrahydro-2-methyl-	102	C5H10S	001795-09-1	43
3	2-(3-Carboxypropionylamino)thiazole	202	C7H10N2O3S	342021-94-7	38
4	1-Butene, 1-(methylthio)-, (Z)-	102	C5H10S	017414-15-2	38
5	3-Ethylthio-1-propene	102	C5H10S	005296-62-8	37





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ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP2-41720:23-41718

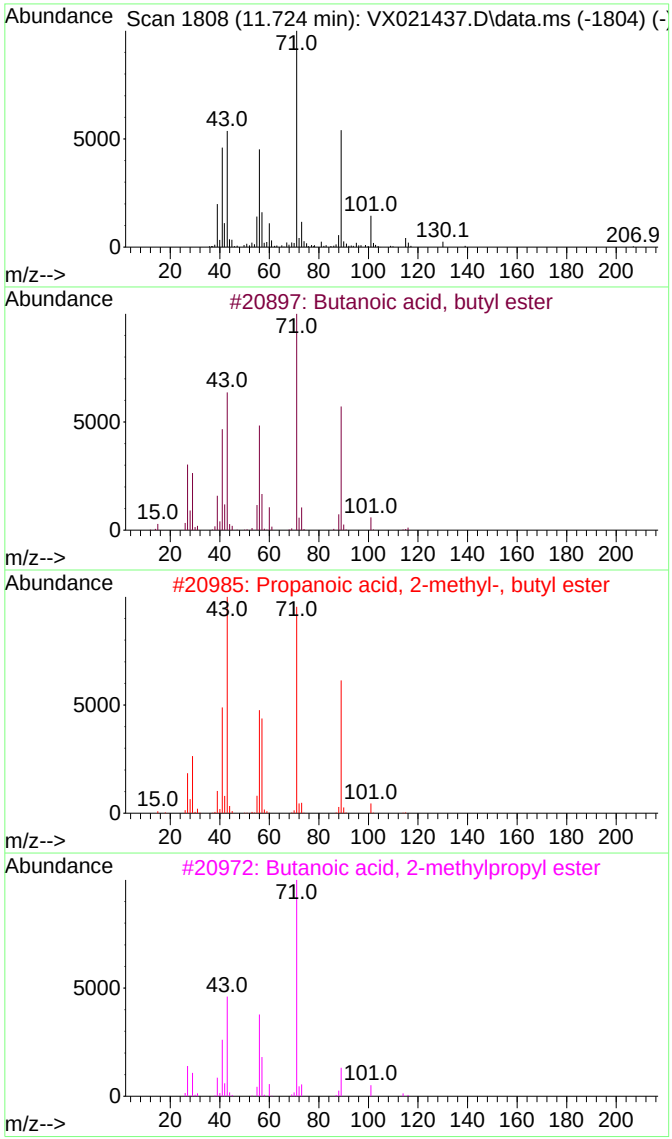
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

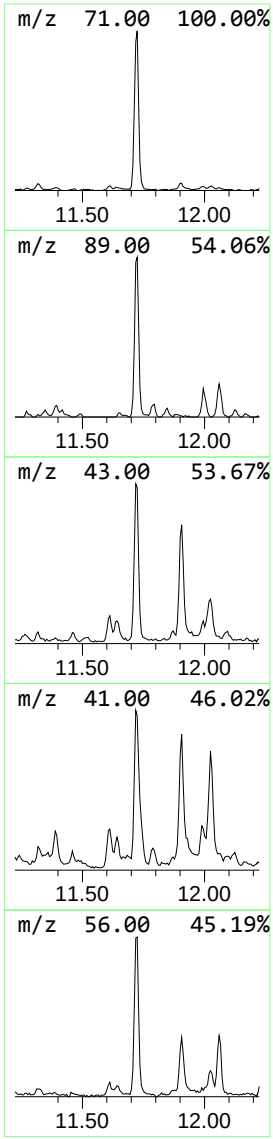
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Butanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.724	16.71 ug/l	119852	1,4-Dichlorobenzene-d4	12.065

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	64
3	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	59
4	Propanoic acid, 2-methyl-, octyl...	200	C12H24O2	000109-15-9	53
5	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	50





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MSVOA_X
ClientSampleId :
COMP2-41720:23-41718

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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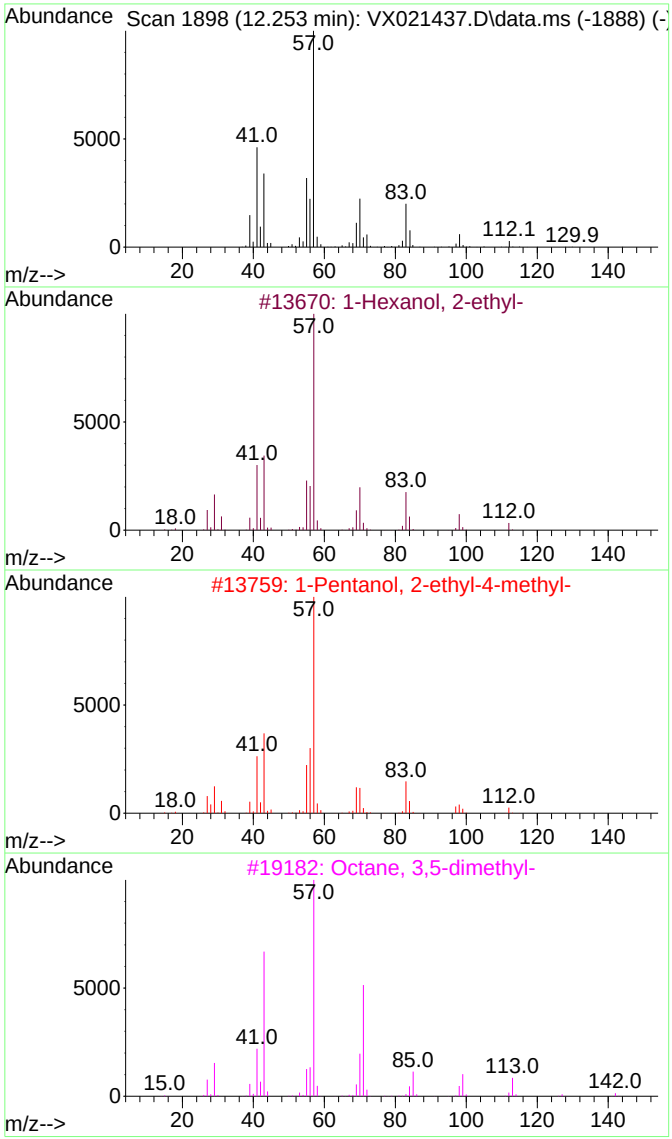
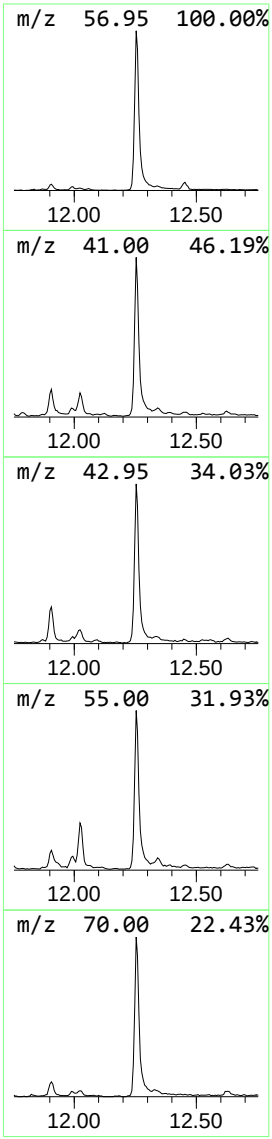
****
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.253	62.53 ug/l	448623	1,4-Dichlorobenzene-d4	12.065

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	64
3	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	50
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	45





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MSVOA_X
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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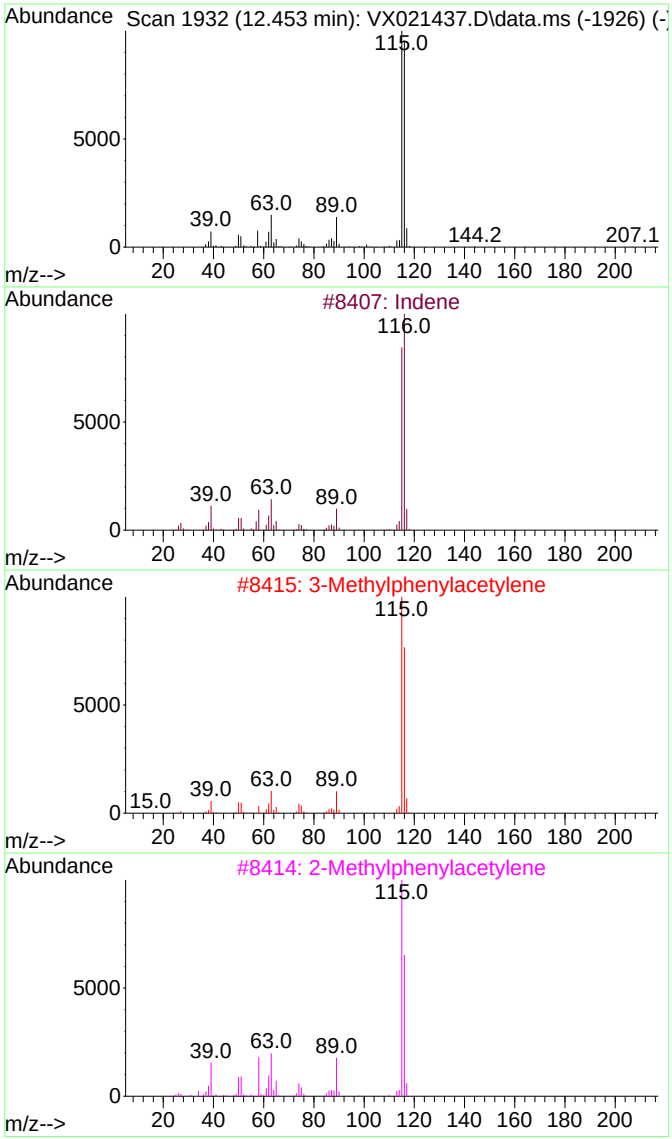
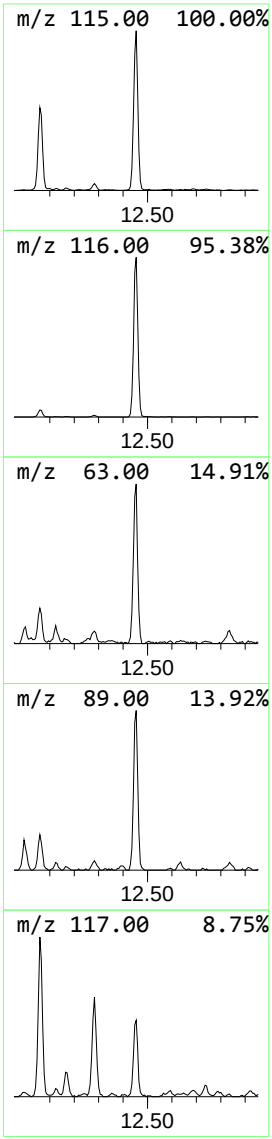
****

Peak Number 7 Indene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.454	29.27 ug/l	210017	1,4-Dichlorobenzene-d4	12.065

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	95
2	3-Methylphenylacetylene	116	C9H8	000766-82-5	94
3	2-Methylphenylacetylene	116	C9H8	000766-47-2	91
4	Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
5	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91





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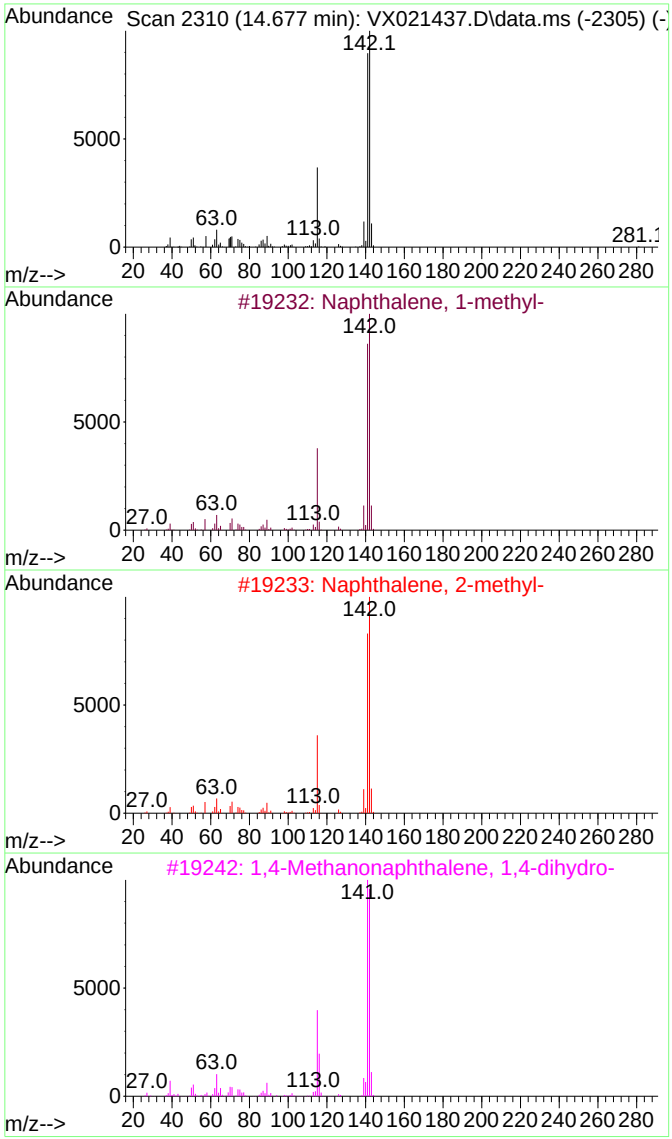
Quant Title : SW846 8260

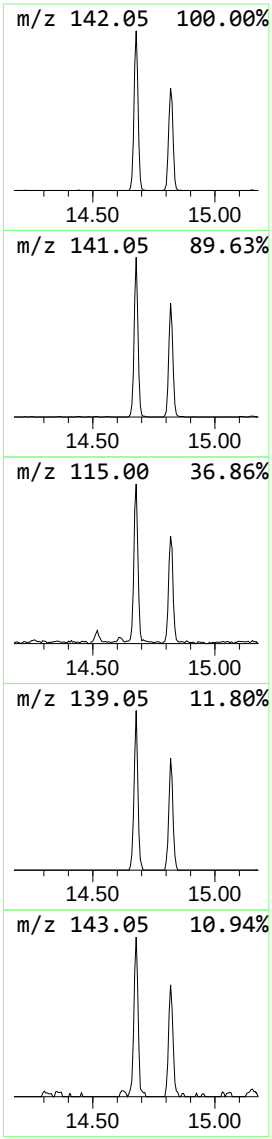
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Naphthalene, 1-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.677	15.38 ug/l	110373	1,4-Dichlorobenzene-d4	12.065

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4	Benzocycloheptatriene	142	C11H10	000264-09-5	90
5	Naphthalene, 1-[(2-propenyloxy)m...	198	C14H14O	074685-39-5	78





Tentatively Identified Compound (LSC) summary

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Data File : VX021437.D
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Instrument : MSVOA_X
ClientSampleId : COMP2-41720:23-41718

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Acetaldehyde	1.470	2370.4	ug/l	10474300	1	5.635	220944	50.0
Ethanol	2.099	36.2	ug/l	160093	1	5.635	220944	50.0
Thiophene, tetr...	9.530	57.1	ug/l	469071	3	10.094	410444	50.0
Thiophene, tetr...	10.447	12.8	ug/l	105010	3	10.094	410444	50.0
Butanoic acid, ...	11.724	16.7	ug/l	119852	4	12.065	358709	50.0
1-Hexanol, 2-et...	12.253	62.5	ug/l	448623	4	12.065	358709	50.0
Indene	12.454	29.3	ug/l	210017	4	12.065	358709	50.0
Naphthalene, 1-...	14.677	15.4	ug/l	110373	4	12.065	358709	50.0