LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051523\
Data File : VX035659.D
Acq On : 15 May 2023 12:53
Operator : JC/MD
Sample : 02751-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-01-70-05052023

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\82X051123W.M
Title : SW846 8260

Signal : TIC: VX035659.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.459	57	61	67	rBV	27684	36199	1.23%	0.287%
2	2.294	192	198	209	rVB	133678	219828	7.48%	1.741%
3	4.233	507	516	525	rBV4	10689	30273	1.03%	0.240%
4	5.385	694	705	719	rBV	136161	395748	13.47%	3.135%
5	5.550	720	732	745	rVB	232179	645913	21.98%	5.116%
6	5.958	788	799	812	rBV	166490	440748	15.00%	3.491%
7	6.757	919	930	948	rVB	373695	897071	30.53%	7.105%
8	7.123	979	990	1007	rBV	697236	1527517	51.98%	12.099%
9	7.574	1055	1064	1078	rBV	131960	262877	8.95%	2.082%
10	8.647	1232	1240	1248	rBV	771164	1209635	41.16%	9.581%
11	9.519	1377	1383	1400	rBV	2211647	2938505	100.00%	23.275%
12	10.055	1464	1471	1482	rBV	800951	1105522	37.62%	8.757%
13	10.854	1597	1602	1616	rVB	117556	143515	4.88%	1.137%
14	11.079	1633	1639	1648	rVB	704105	887929	30.22%	7.033%
15	11.616	1717	1727	1732	rBV2	53038	72652	2.47%	0.575%
16	11.927	1774	1778	1788	rVB	94011	115745	3.94%	0.917%
17	12.018	1788	1793	1801	rBV	874737	1085198	36.93%	8.596%
18	12.445	1857	1863	1870	rBV2	20599	31056	1.06%	0.246%
19	12.591	1882	1887	1901	rBV	134667	188479	6.41%	1.493%
20	12.853	1925	1930	1938	rBV	38542	48352	1.65%	0.383%
21	13.463	2026	2030	2035	rBV2	21248	29483	1.00%	0.234%
22	14.256	2154	2160	2177	rBV	114258	194582	6.62%	1.541%
23	14.999	2276	2282	2293	rBV4	21817	39364	1.34%	0.312%
24	15.542	2362	2371	2377	rBV2	26616	43419	1.48%	0.344%
25	16.469	2516	2523	2532	rVB2	19265	35447	1.21%	0.281%

Sum of corrected areas: 12625057

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Instrument :
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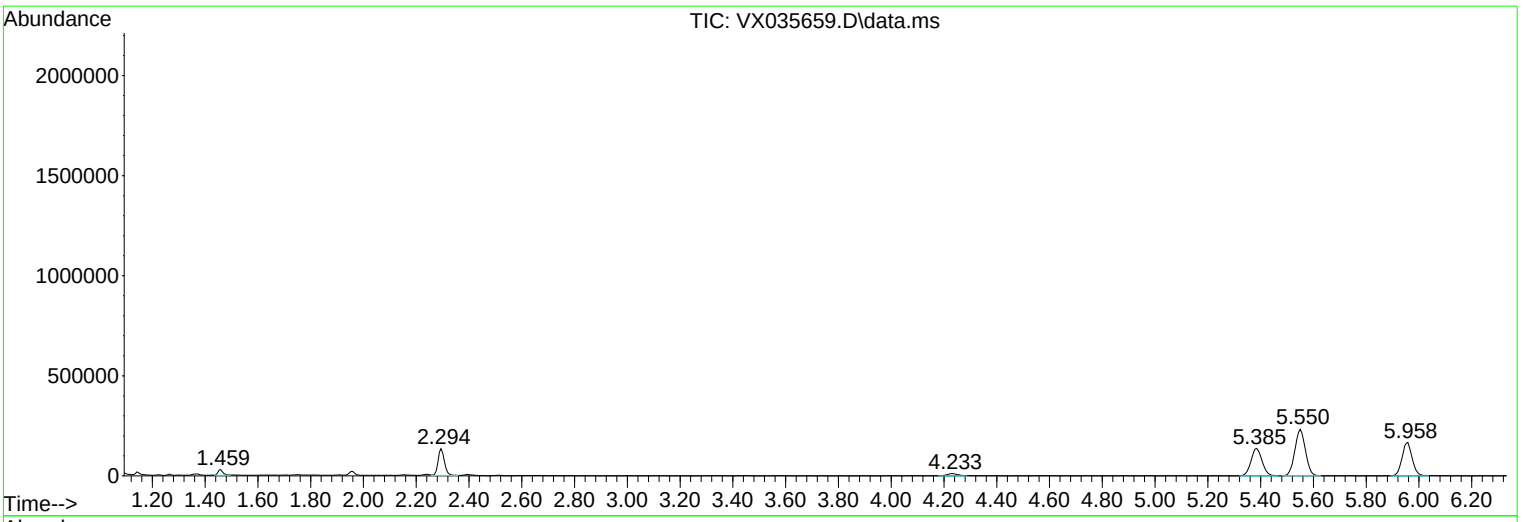
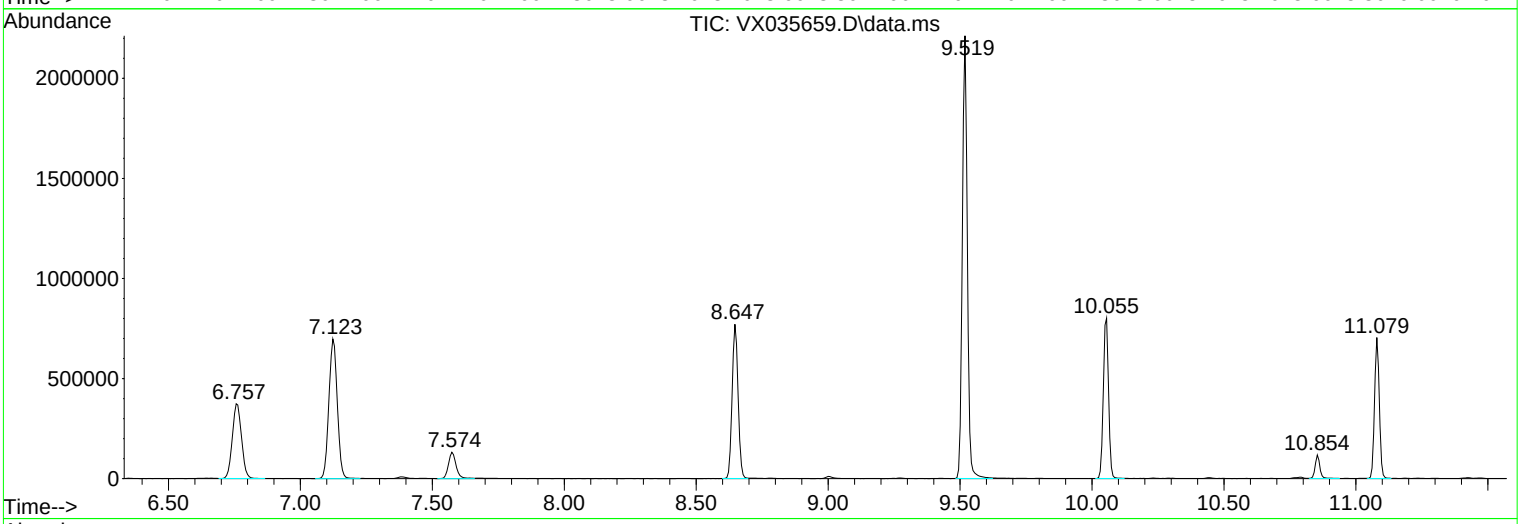
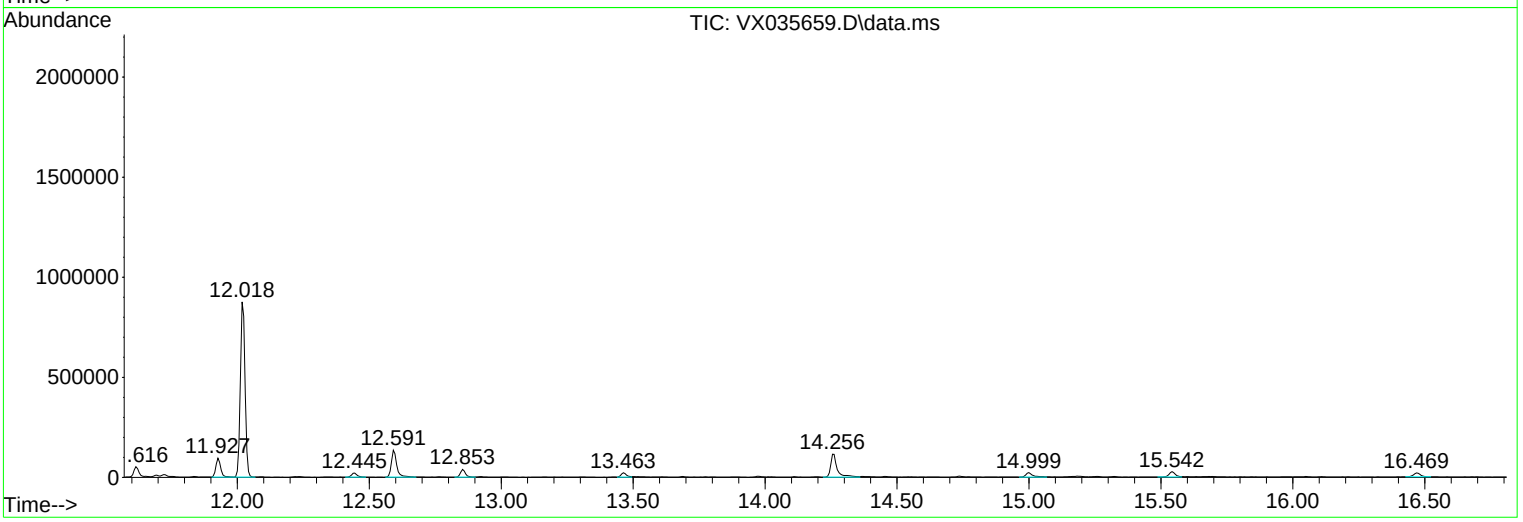
ClientSampleId :
FSND-PRO-01-70-05052023

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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







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Data File : VX035659.D
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FSND-PRO-01-70-05052023

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

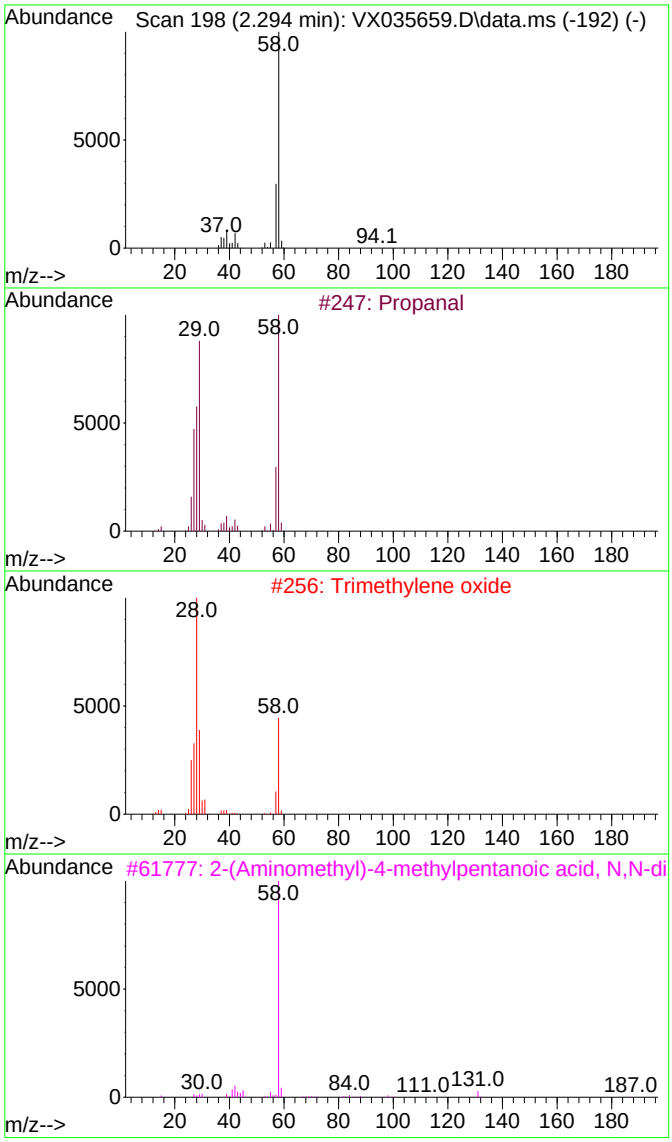
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

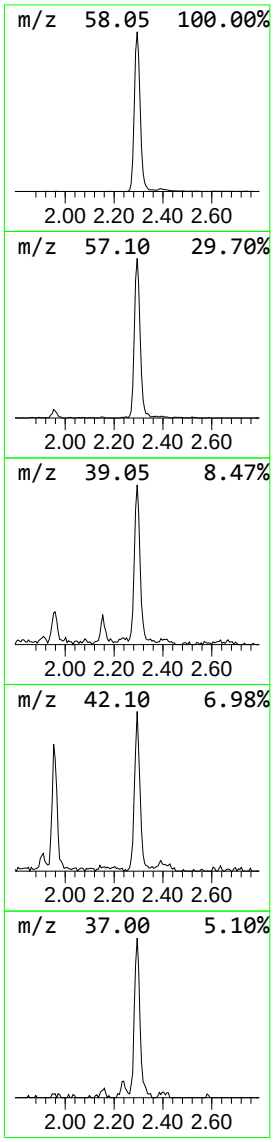
****

Peak Number 1 Propanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.294	17.02 ug/l	219828	Pentafluorobenzene	5.550

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	78
2	Trimethylene oxide	58	C3H6O	000503-30-0	9
3	2-(Aminomethyl)-4-methylpentanoi...	187	C10H21NO2	1891211-54-3	9
4	Propylene oxide	58	C3H6O	000075-56-9	7
5	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	7





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Data File : VX035659.D
Acq On : 15 May 2023 12:53
Operator : JC/MD
Sample : 02751-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-01-70-05052023

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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

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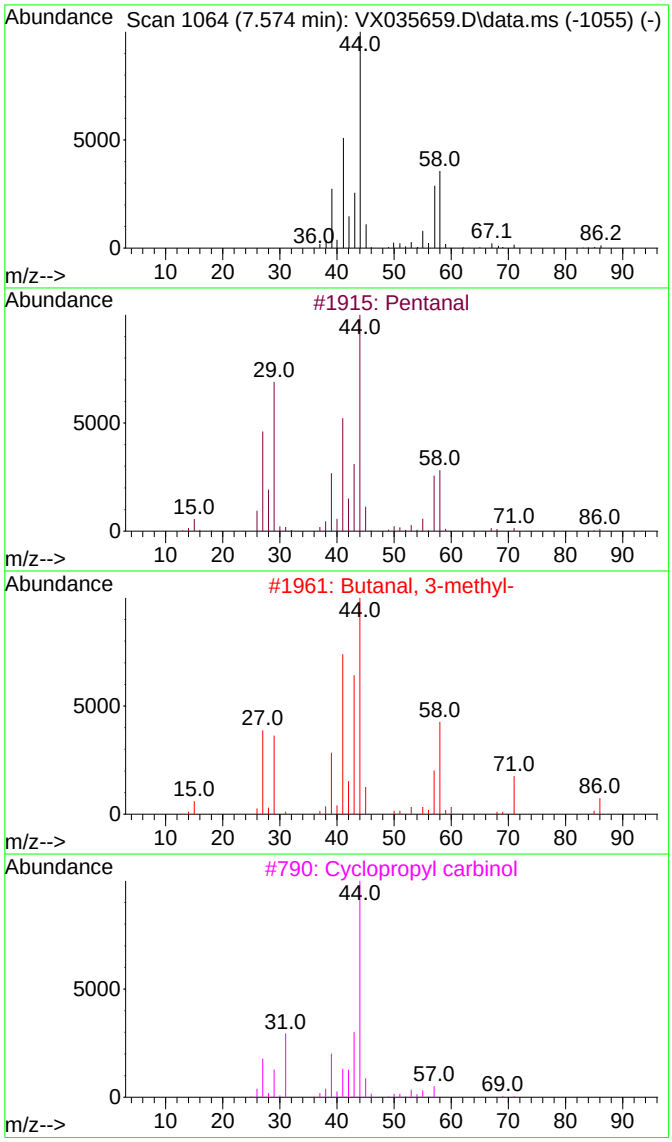
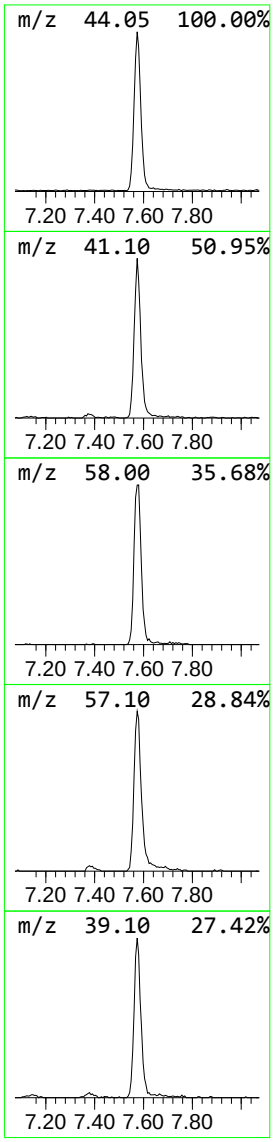
Peak Number 2 Pentanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.574	14.65 ug/l	262877	1,4-Difluorobenzene	6.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	91
2	Butanal, 3-methyl-	86	C5H10O	000590-86-3	74
3	Cyclopropyl carbinol	72	C4H8O	002516-33-8	45
4	1-Octadecanamine, N-methyl-	283	C19H41N	002439-55-6	43
5	2-Propanamine	59	C3H9N	000075-31-0	9





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Data File : VX035659.D
Acq On : 15 May 2023 12:53
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-01-70-05052023

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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

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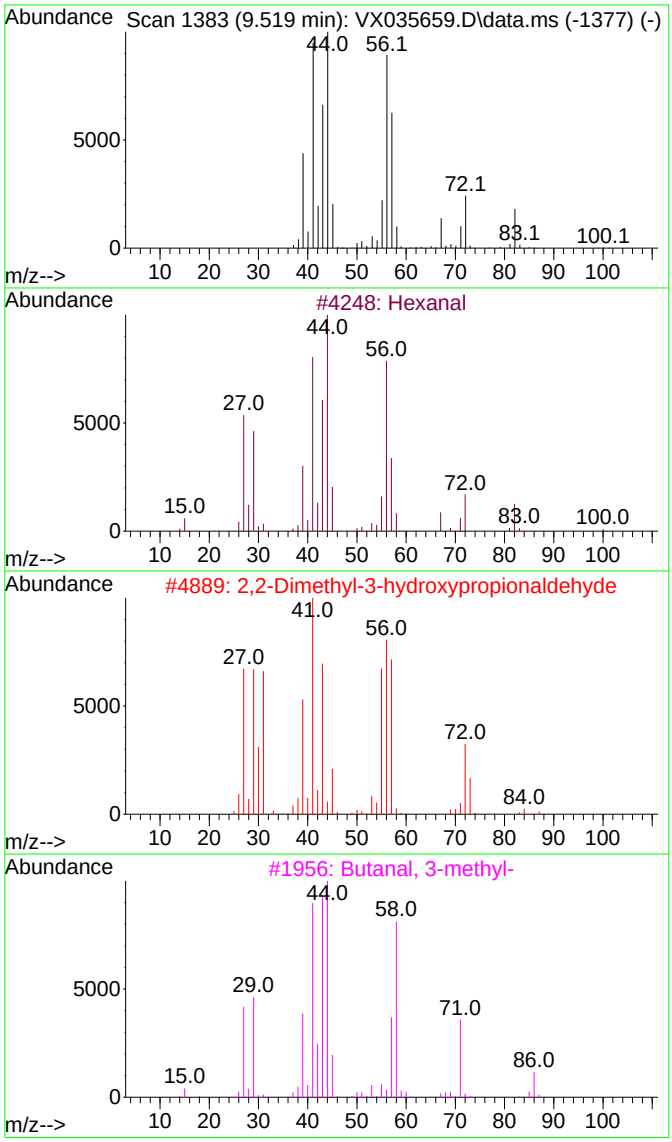
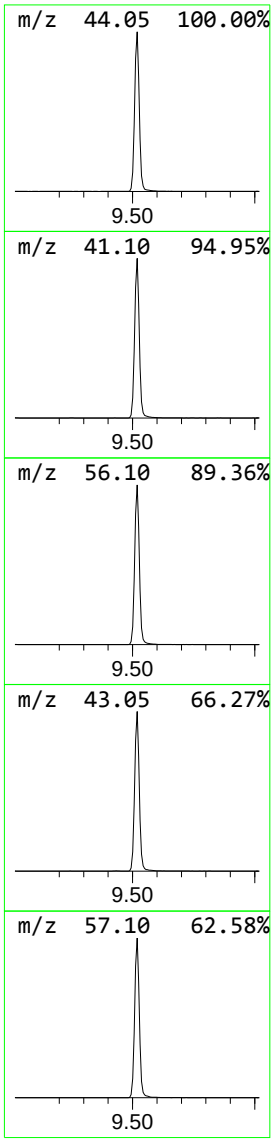
Peak Number 3 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.519	132.90 ug/l	2938510	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	80
2	2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	37
3	Butanal, 3-methyl-	86	C5H10O	000590-86-3	32
4	Glutaraldehyde	100	C5H8O2	000111-30-8	30
5	Butanal	72	C4H8O	000123-72-8	27





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Operator : JC/MD
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-01-70-05052023

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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

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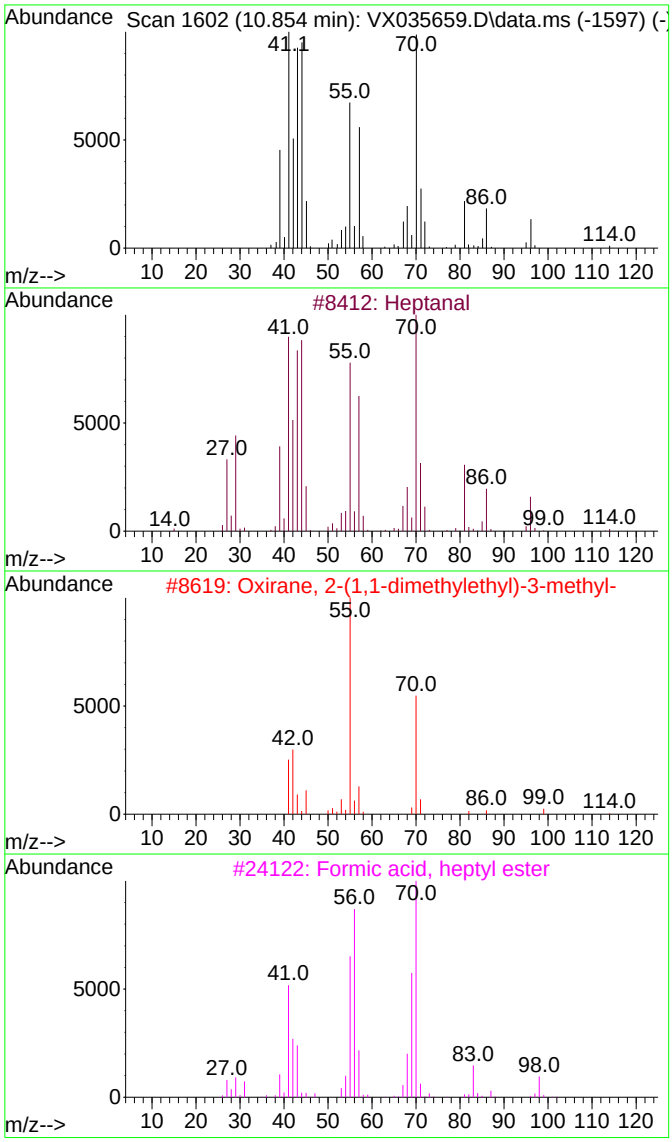
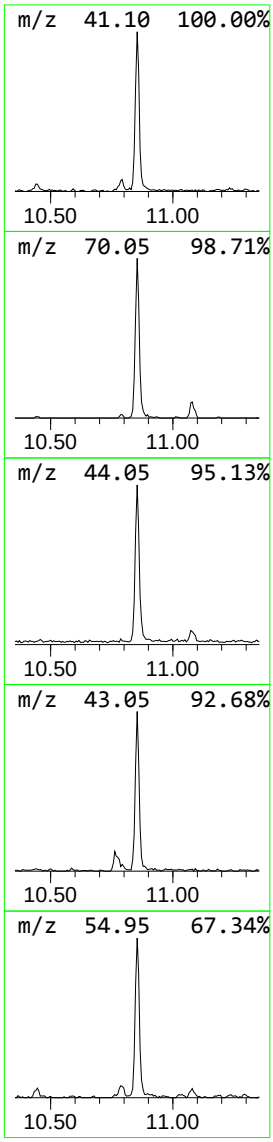
Peak Number 4 Heptanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.854	6.49 ug/l	143515	Chlorobenzene-d5	10.055

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal	114	C7H14O	000111-71-7	98
2	Oxirane, 2-(1,1-dimethylethyl)-3...	114	C7H14O	053897-30-6	38
3	Formic acid, heptyl ester	144	C8H16O2	000112-23-2	27
4	1-Heptene	98	C7H14	000592-76-7	22
5	Hexanal, 4-methyl-	114	C7H14O	041065-97-8	22





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX051523\
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Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-01-70-05052023

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

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

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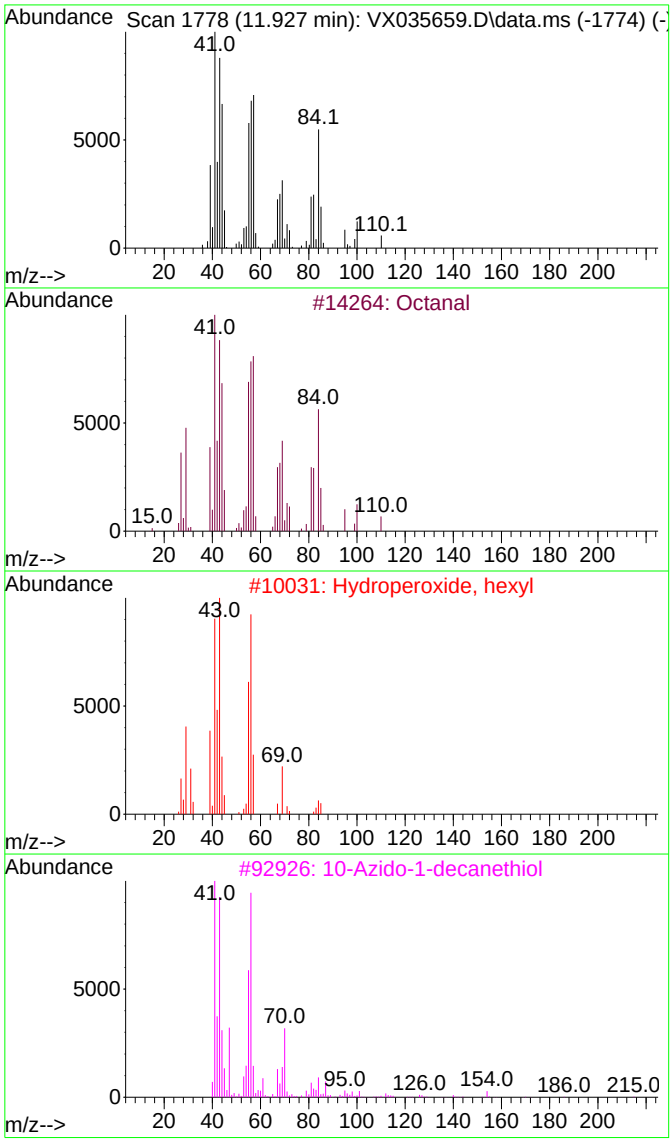
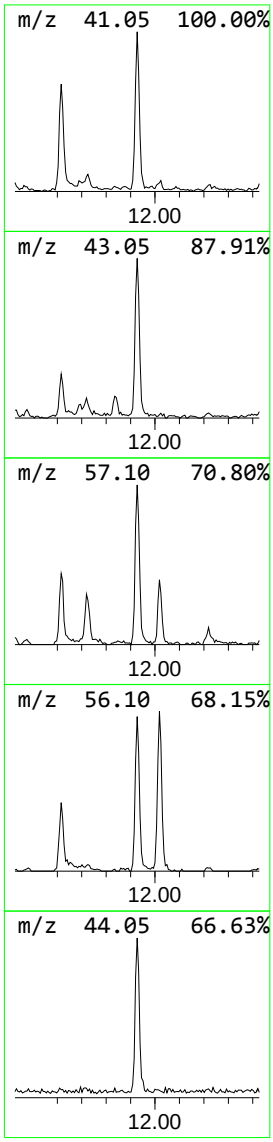
Peak Number 5 Octanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.927	5.33 ug/l	115745	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal	128	C8H16O	000124-13-0	91
2	Hydroperoxide, hexyl	118	C6H14O2	004312-76-9	38
3	10-Azido-1-decanethiol	215	C10H21N3S	1152113-44-4	35
4	Cyclopentanol, 2-methyl-, trans-	100	C6H12O	025144-04-1	30
5	Cyclopentanol, 2-methyl-	100	C6H12O	024070-77-7	27





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Instrument :
MSVOA_X
ClientSampleId :
FSND-PRO-01-70-05052023

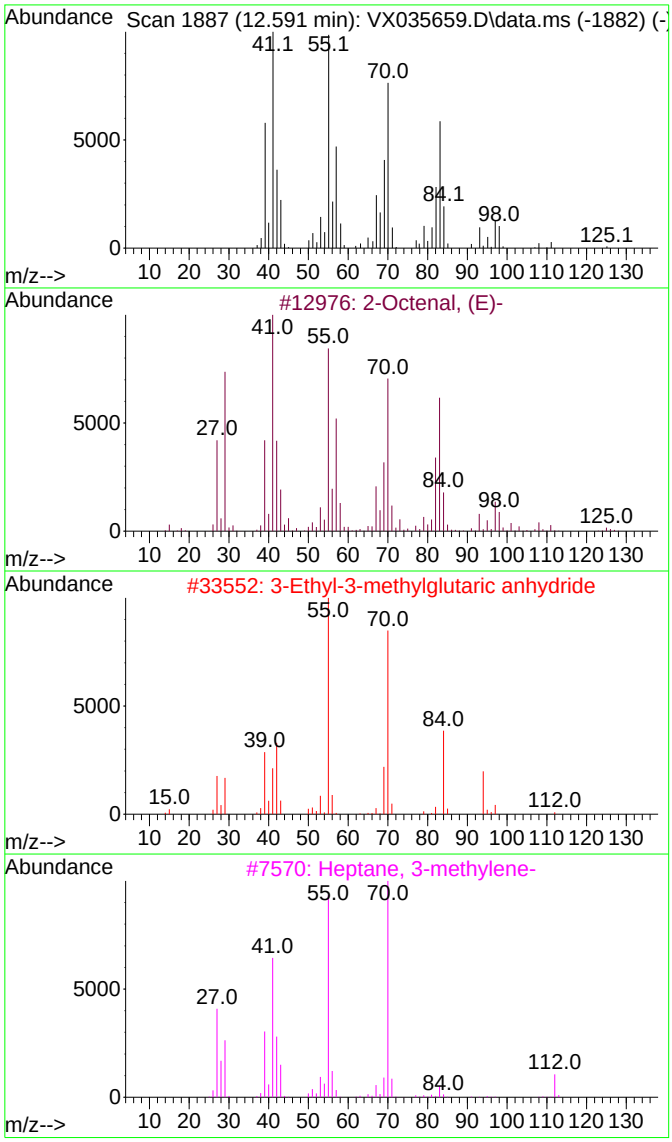
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X051123W.M
Quant Title : SW846 8260

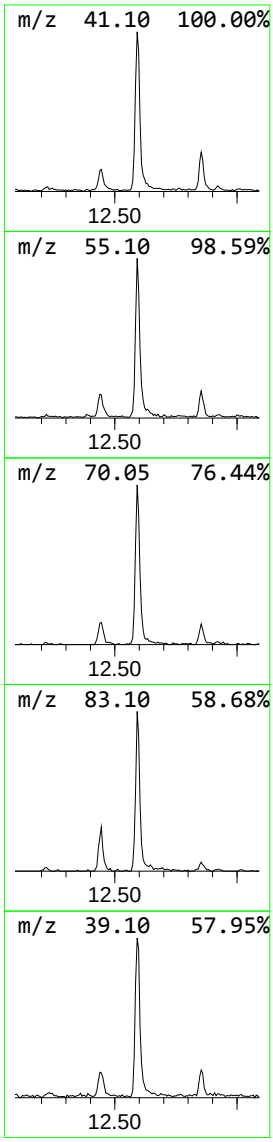
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-Octenal, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.591	8.68 ug/l	188479	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octenal, (E)-	126	C8H14O	002548-87-0	90
2	3-Ethyl-3-methylglutaric anhydride	156	C8H12O3	006970-57-6	43
3	Heptane, 3-methylene-	112	C8H16	001632-16-2	38
4	5-Oxa-6-azaspiro[3.4]oct-6-ene	111	C6H9NO	1000362-18-0	25
5	2-Butenal, (E)-	70	C4H6O	000123-73-9	25





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Quant Title : SW846 8260

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

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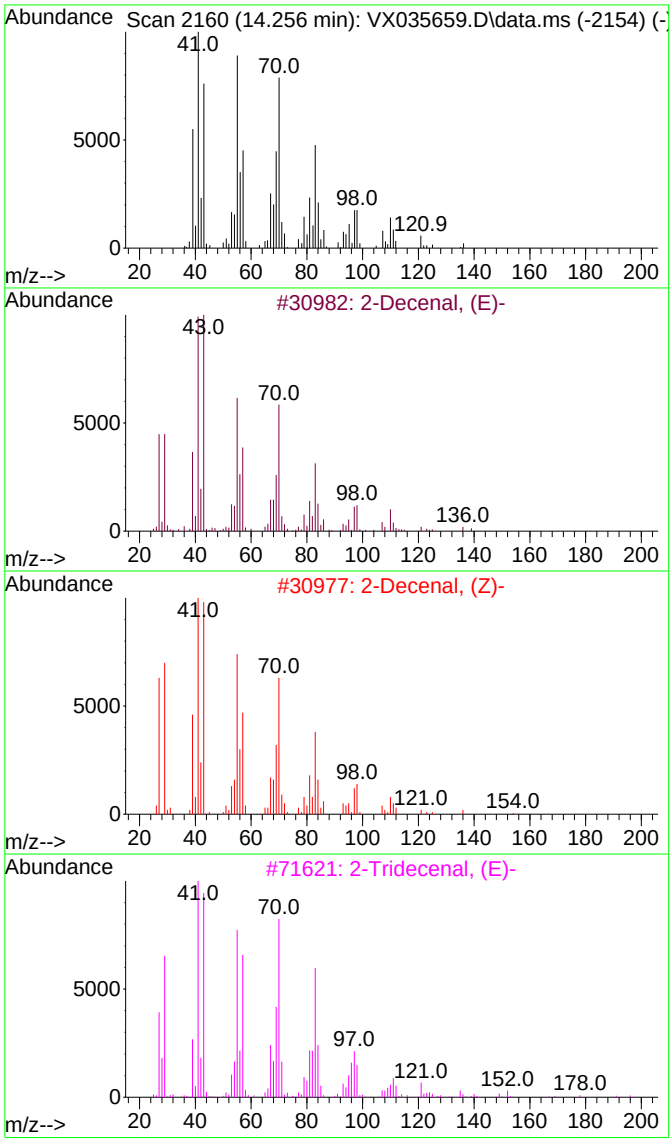
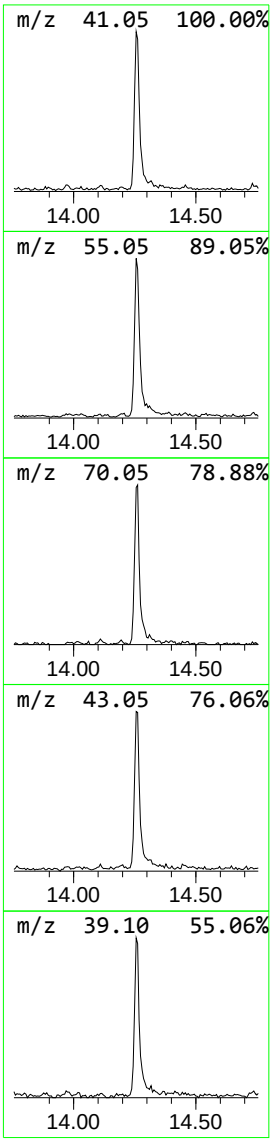
Peak Number 7 2-Decenal, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.256	8.97 ug/l	194582	1,4-Dichlorobenzene-d4	12.018

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Decenal, (E)-	154	C10H18O	003913-81-3	72
2	2-Decenal, (Z)-	154	C10H18O	002497-25-8	72
3	2-Tridecenal, (E)-	196	C13H24O	007069-41-2	64
4	2-Methylene cyclopentanol	98	C6H10O	020461-31-8	53
5	Octane, 2-chloro-	148	C8H17Cl	000628-61-5	47





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propanal	2.294	17.0	ug/l	219828	1	5.550	645913	50.0
Pentanal	7.574	14.7	ug/l	262877	2	6.763	897071	50.0
Hexanal	9.519	132.9	ug/l	2938510	3	10.055	1105520	50.0
Heptanal	10.854	6.5	ug/l	143515	3	10.055	1105520	50.0
Octanal	11.927	5.3	ug/l	115745	4	12.018	1085200	50.0
2-Octenal, (E)-	12.591	8.7	ug/l	188479	4	12.018	1085200	50.0
2-Decenal, (E)-	14.256	9.0	ug/l	194582	4	12.018	1085200	50.0