LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012022\
Data File : VU046805.D
Acq On : 20 Jan 2022 12:46
Operator : SY/MD
Sample : N1194-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXX2

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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_U\Method\SFAMUTR011822WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU046805.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	22	rVB	57646	57945	7.28%	1.066%
2	1.472	36	41	54	rVB2	27011	31313	3.93%	0.576%
3	1.600	70	81	90	rBV3	59188	86918	10.91%	1.599%
4	1.919	170	180	198	rVB	36864	51409	6.46%	0.946%
5	2.157	244	254	262	rVB4	5031	8086	1.02%	0.149%
6	2.208	262	270	291	rVB5	4739	9680	1.22%	0.178%
7	2.578	367	385	399	rBV4	127166	259801	32.62%	4.779%
8	3.874	770	788	818	rVB	137510	334265	41.98%	6.149%
9	4.645	1012	1028	1082	rBV	46009	185954	23.35%	3.421%
10	5.066	1136	1159	1185	rBV	68722	158323	19.88%	2.912%
11	5.321	1224	1238	1253	rVB3	16704	37023	4.65%	0.681%
12	5.729	1343	1365	1382	rBV3	132584	350501	44.01%	6.448%
13	6.250	1514	1527	1544	rBV	108432	205621	25.82%	3.782%
14	6.546	1603	1619	1640	rBV	422507	796340	100.00%	14.649%
15	6.693	1652	1665	1682	rVB	82713	160930	20.21%	2.960%
16	6.883	1711	1724	1739	rBV2	15156	29907	3.76%	0.550%
17	7.568	1924	1937	1957	rBV	42027	73453	9.22%	1.351%
18	7.899	2027	2040	2054	rBV	162814	281681	35.37%	5.182%
19	8.182	2117	2128	2142	rBV2	25724	43533	5.47%	0.801%
20	8.555	2234	2244	2253	rBV3	14271	22981	2.89%	0.423%
21	8.635	2256	2269	2296	rBV	252900	457460	57.45%	8.415%
22	8.787	2305	2316	2343	rVB	150160	265462	33.34%	4.883%
23	9.420	2500	2513	2538	rBV	170065	282472	35.47%	5.196%
24	10.346	2791	2801	2817	rVB	29940	47876	6.01%	0.881%
25	10.758	2918	2929	2945	rBV	76821	123037	15.45%	2.263%
26	11.259	3071	3085	3091	rBV	10933	14914	1.87%	0.274%
27	11.298	3091	3097	3106	rVB3	5653	8342	1.05%	0.153%
28	11.690	3207	3219	3232	rBV2	72276	110285	13.85%	2.029%
29	11.812	3245	3257	3274	rVB	201284	322016	40.44%	5.924%
30	12.195	3364	3376	3391	rBV	166306	271327	34.07%	4.991%
31	12.549	3478	3486	3496	rBV6	5805	9292	1.17%	0.171%
32	12.889	3581	3592	3609	rBV	222899	328131	41.20%	6.036%
33	14.735	4159	4166	4175	rBV5	7118	9951	1.25%	0.183%

Sum of corrected areas: 5436229

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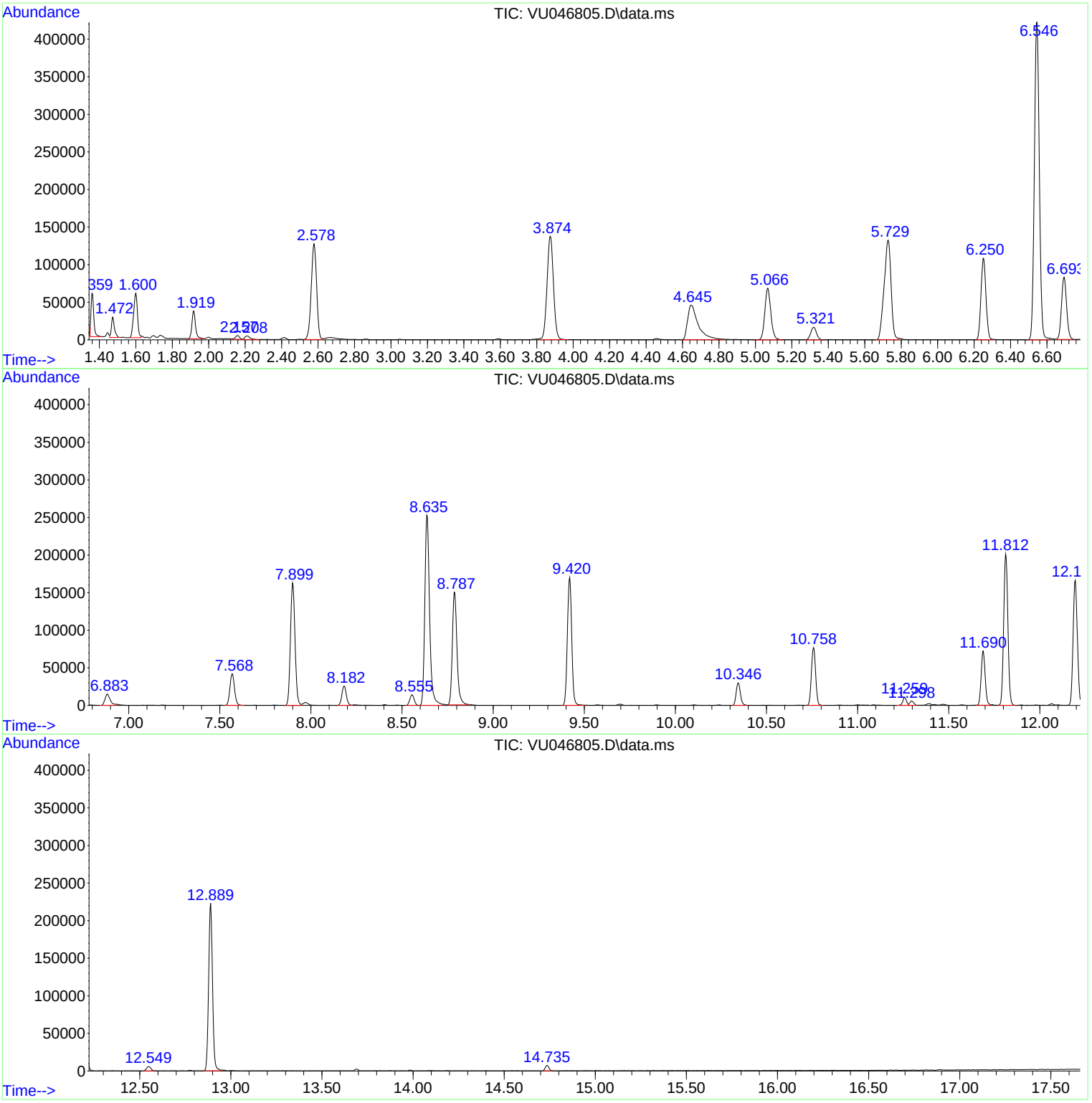
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXX2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Data File : VU046805.D
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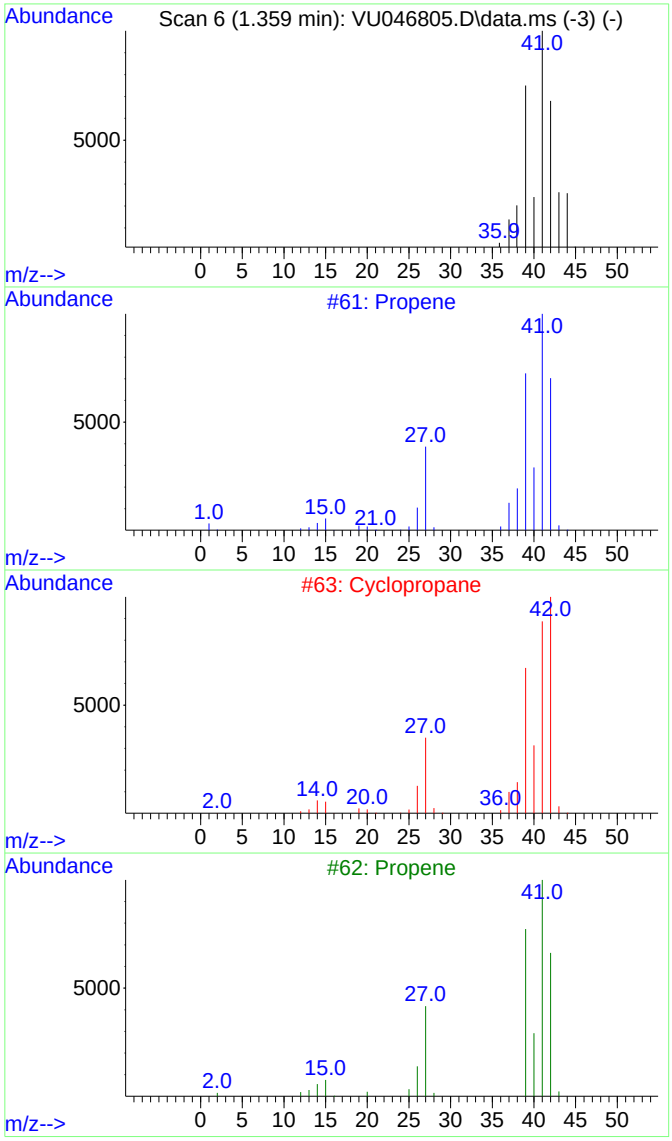
Quant Title : TRACE VOA SFAM1.0

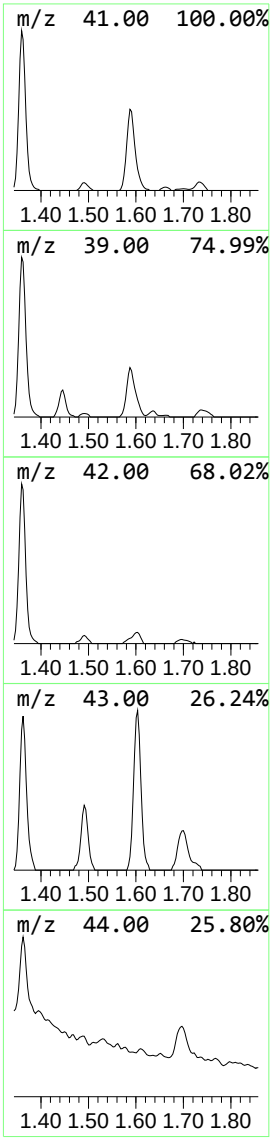
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.359	1.41 ug/L	57945	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	90
2	Cyclopropane	42	C3H6	000075-19-4	64
3	Propene	42	C3H6	000115-07-1	42
4	Cyclopropane	42	C3H6	000075-19-4	9
5	Cyclopropane	42	C3H6	000075-19-4	9





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Data File : VU046805.D
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Operator : SY/MD
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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXX2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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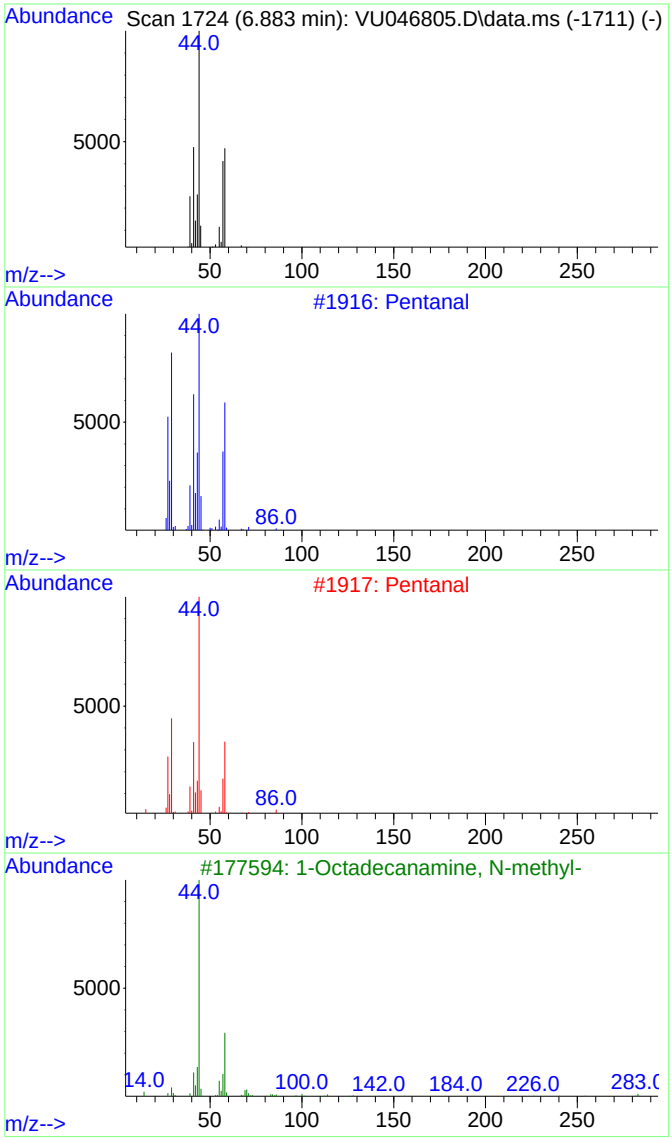
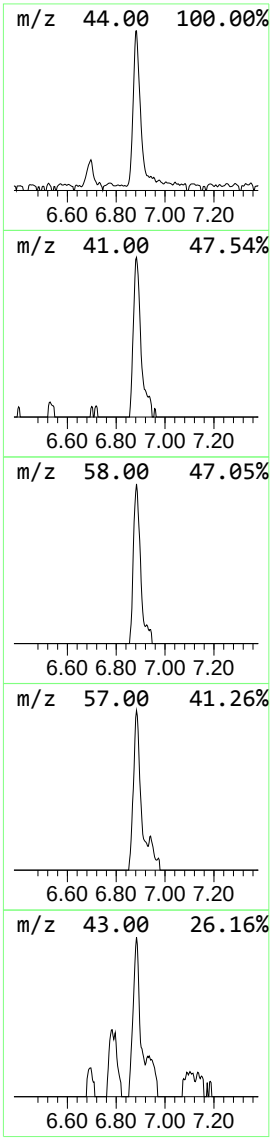
Peak Number 3 Pentanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.883	0.73 ug/L	29907	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	78
2	Pentanal	86	C5H10O	000110-62-3	64
3	1-Octadecanamine, N-methyl-	283	C19H41N	002439-55-6	9
4	Cyclopropyl carbinol	72	C4H8O	002516-33-8	9
5	Ethylene oxide	44	C2H4O	000075-21-8	5





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Data File : VU046805.D
Acq On : 20 Jan 2022 12:46
Operator : SY/MD
Sample : N1194-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXX2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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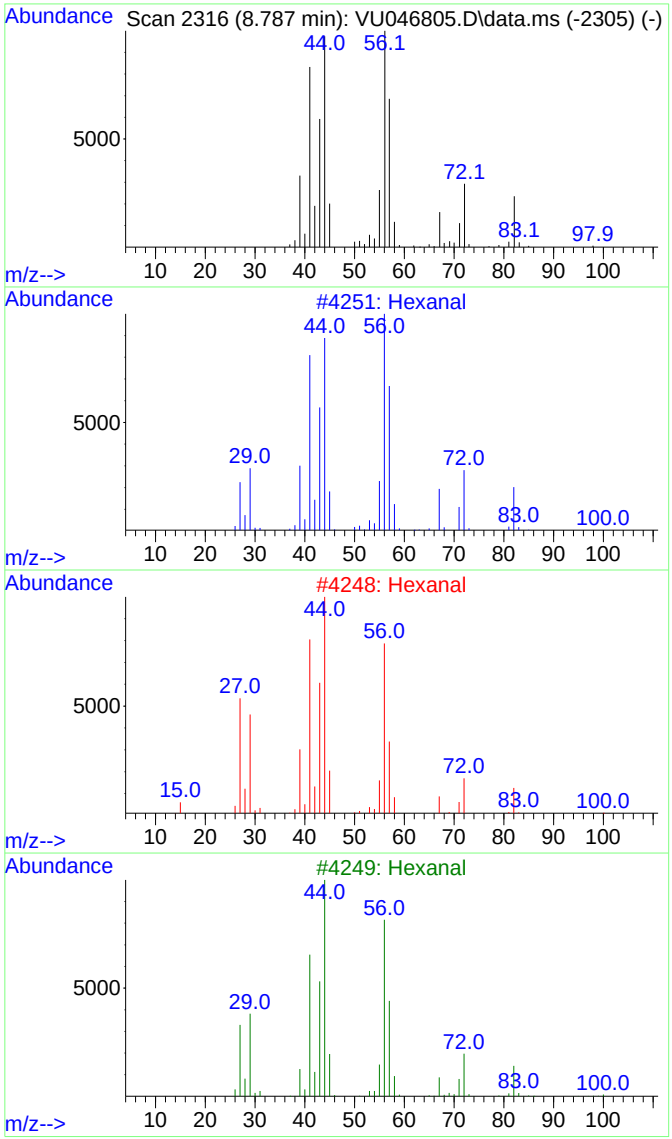
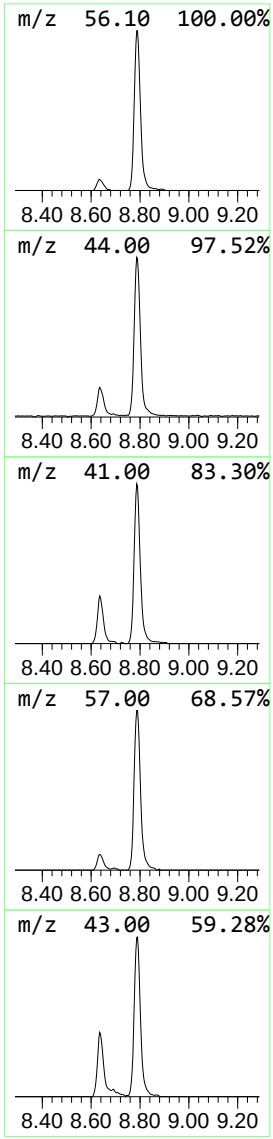
Peak Number 5 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.787	4.70 ug/L	265462	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	90
2	Hexanal	100	C6H12O	000066-25-1	83
3	Hexanal	100	C6H12O	000066-25-1	83
4	Hexanal	100	C6H12O	000066-25-1	83
5	Hexanal	100	C6H12O	000066-25-1	78





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Acq On : 20 Jan 2022 12:46
Operator : SY/MD
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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXX2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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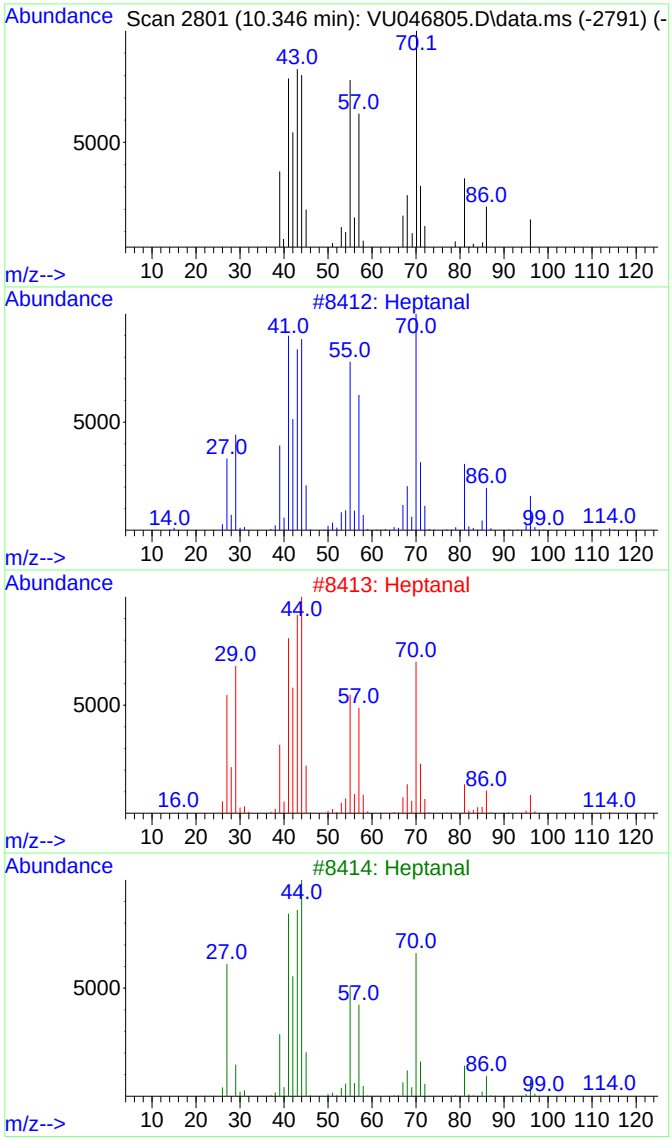
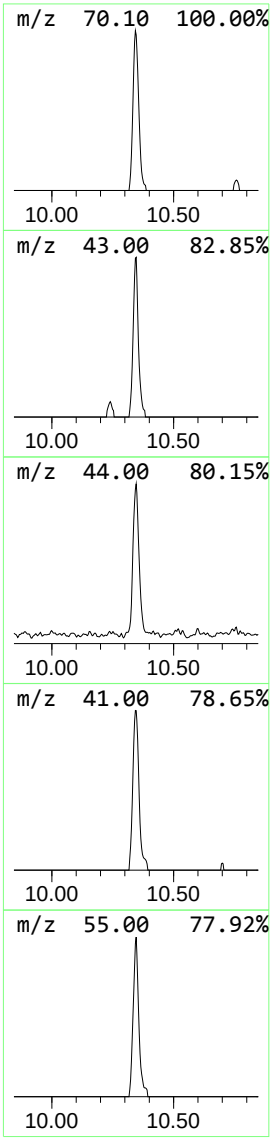
Peak Number 6 Heptanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.346	0.85 ug/L	47876	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal	114	C7H14O	000111-71-7	91
2	Heptanal	114	C7H14O	000111-71-7	90
3	Heptanal	114	C7H14O	000111-71-7	78
4	Heptanal	114	C7H14O	000111-71-7	72
5	Heptanal	114	C7H14O	000111-71-7	59





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Data File : VU046805.D
Acq On : 20 Jan 2022 12:46
Operator : SY/MD
Sample : N1194-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXX2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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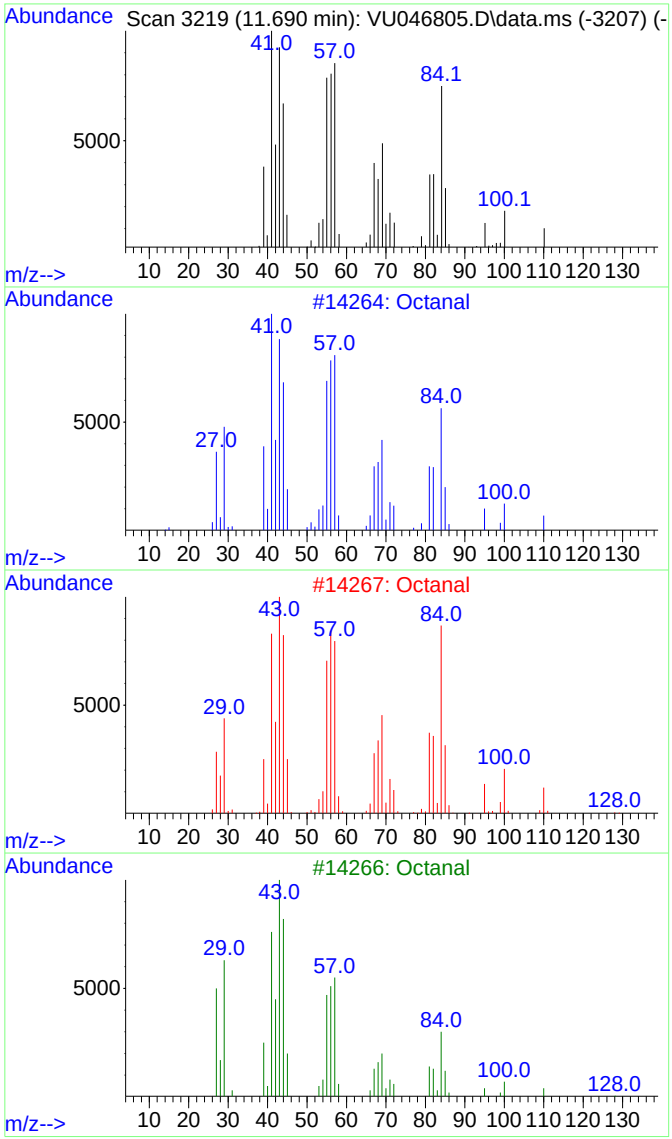
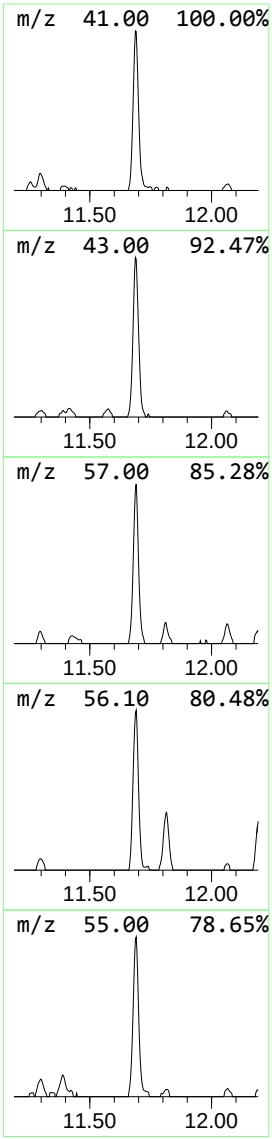
Peak Number 7 Octanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.690	1.71 ug/L	110285	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal	128	C8H16O	000124-13-0	91
2	Octanal	128	C8H16O	000124-13-0	91
3	Octanal	128	C8H16O	000124-13-0	64
4	Octanal	128	C8H16O	000124-13-0	59
5	Octanal	128	C8H16O	000124-13-0	59





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Acq On : 20 Jan 2022 12:46
Operator : SY/MD
Sample : N1194-02
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXX2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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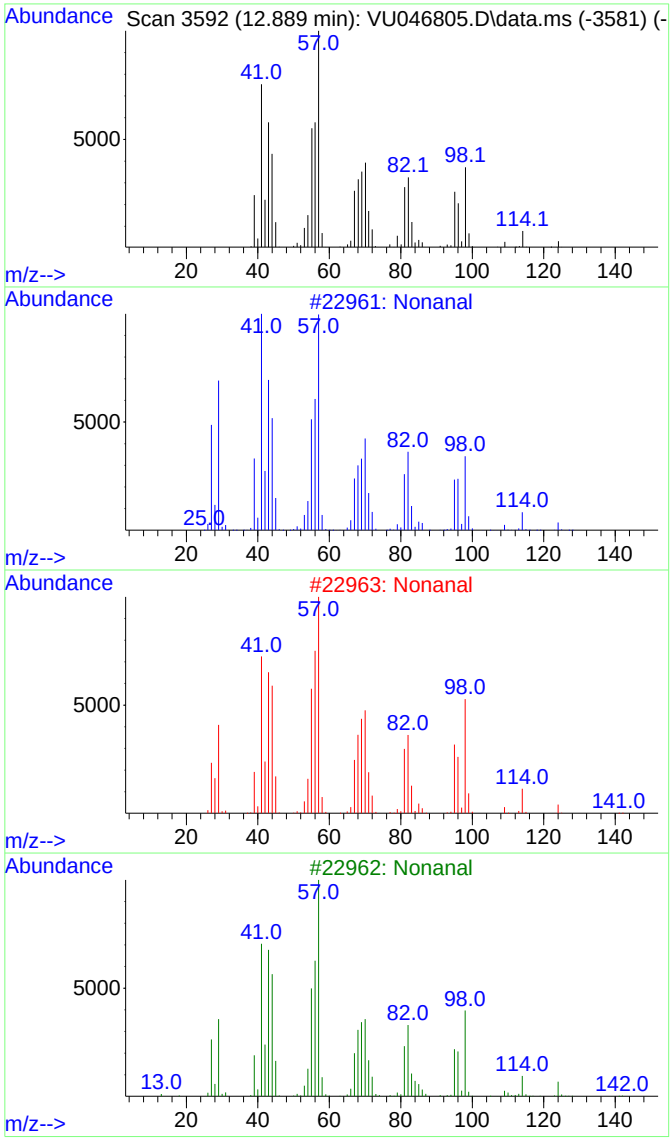
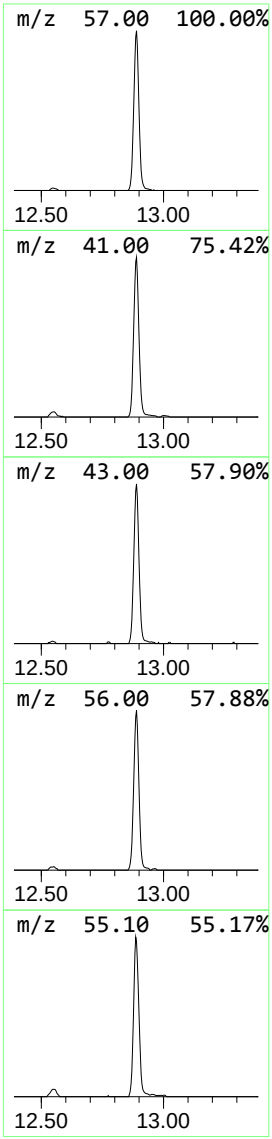
Peak Number 8 Nonanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.889	5.09 ug/L	328131	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal	142	C9H18O	000124-19-6	91
2	Nonanal	142	C9H18O	000124-19-6	91
3	Nonanal	142	C9H18O	000124-19-6	86
4	Nonanal	142	C9H18O	000124-19-6	83
5	Heptane, 2-chloro-	134	C7H15Cl	001001-89-4	27





Tentatively Identified Compound (LSC) summary

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Quant Title : TRACE VOA SFAM1.0

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL) Alkane: S...	1.359	1.4	ug/L	57945	1	6.250	205621	5.0
Pentanal	6.883	0.7	ug/L	29907	1	6.250	205621	5.0
Hexanal	8.787	4.7	ug/L	265462	2	9.420	282472	5.0
Heptanal	10.346	0.8	ug/L	47876	2	9.420	282472	5.0
Octanal	11.690	1.7	ug/L	110285	3	11.812	322016	5.0
Nonanal	12.889	5.1	ug/L	328131	3	11.812	322016	5.0