LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011922\
Data File : VU046797.D
Acq On : 19 Jan 2022 14:36
Operator : SY/MD
Sample : N1194-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXX1

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: VU046797.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	70	81	90	rBV2	72158	98425	1.86%	0.710%
2	1.919	171	180	199	rVB	49549	67961	1.28%	0.490%
3	2.581	367	386	399	rBV4	219678	456195	8.61%	3.292%
4	3.874	768	788	816	rVB2	244151	586485	11.07%	4.232%
5	4.649	1014	1029	1078	rBV2	54269	227344	4.29%	1.640%
6	5.067	1138	1159	1184	rBV	88292	203088	3.83%	1.465%
7	5.321	1222	1238	1258	rVB2	30963	69383	1.31%	0.501%
8	5.729	1344	1365	1382	rBV2	178410	462804	8.74%	3.339%
9	6.253	1510	1528	1549	rBV	131553	251715	4.75%	1.816%
10	6.546	1602	1619	1643	rBV	579436	1095170	20.67%	7.902%
11	6.694	1652	1665	1691	rVB	109092	215425	4.07%	1.554%
12	6.883	1713	1724	1747	rBV2	27340	58739	1.11%	0.424%
13	7.568	1925	1937	1961	rBV	55805	96237	1.82%	0.694%
14	7.903	2027	2041	2056	rBV	219561	380679	7.19%	2.747%
15	8.134	2099	2113	2121	rBV	62078	103187	1.95%	0.745%
16	8.182	2121	2128	2141	rVB	35022	58287	1.10%	0.421%
17	8.555	2232	2244	2257	rVB	50472	81932	1.55%	0.591%
18	8.639	2257	2270	2304	rBV	326330	644220	12.16%	4.648%
19	8.790	2304	2317	2360	rVB	525163	961744	18.15%	6.939%
20	9.420	2499	2513	2533	rBV	207629	345924	6.53%	2.496%
21	10.346	2790	2801	2825	rBV	134958	223005	4.21%	1.609%
22	10.758	2918	2929	2949	rBV	103016	170175	3.21%	1.228%
23	11.259	3074	3085	3092	rBV	42481	62031	1.17%	0.448%
24	11.690	3207	3219	3233	rBV	484801	715302	13.50%	5.161%
25	11.812	3246	3257	3276	rVB	260873	421574	7.96%	3.042%
26	12.195	3359	3376	3390	rBV	233263	373021	7.04%	2.692%
27	12.889	3578	3592	3624	rBV	3625644	5297719	100.00%	38.226%
28	14.735	4155	4166	4182	rBV2	84987	131305	2.48%	0.947%

Sum of corrected areas: 13859076

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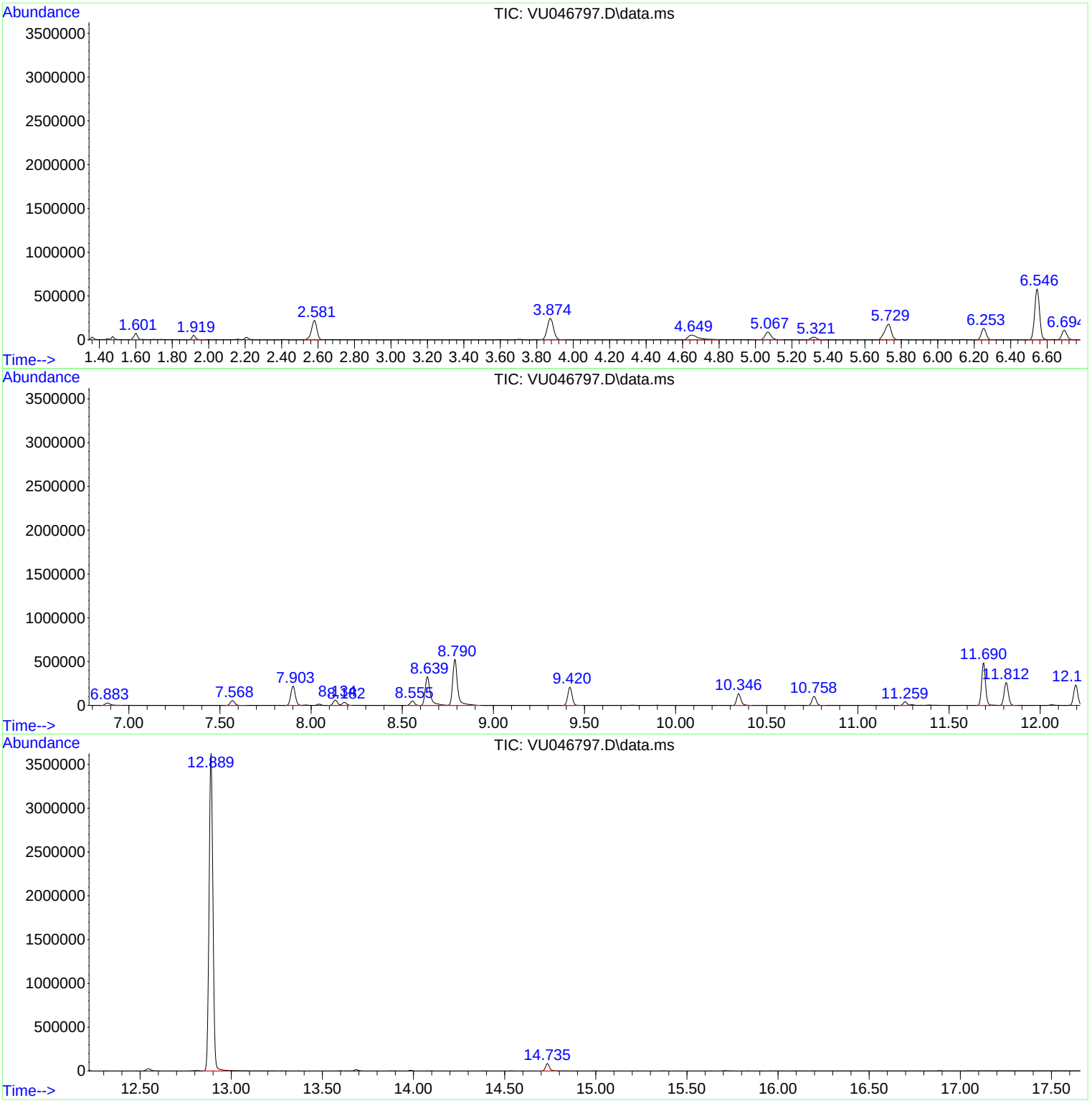
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXX1

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011922\
Data File : VU046797.D
Acq On : 19 Jan 2022 14:36
Operator : SY/MD
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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXX1

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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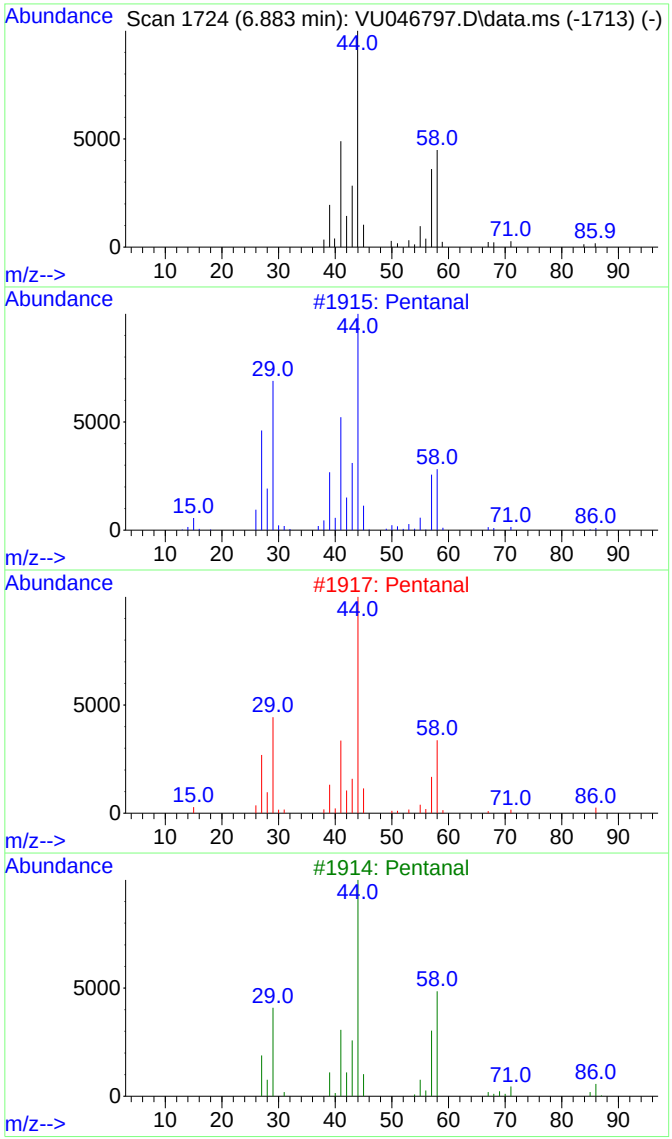
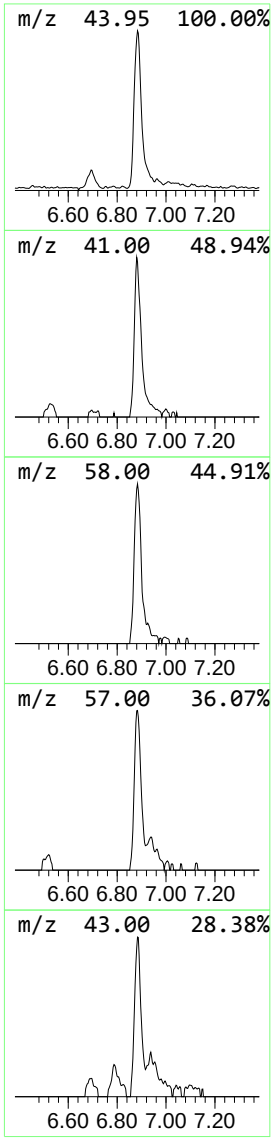
Peak Number 1 Pentanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.883	1.17 ug/L	58739	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	83
2	Pentanal	86	C5H10O	000110-62-3	78
3	Pentanal	86	C5H10O	000110-62-3	56
4	Butanal, 3-methyl-	86	C5H10O	000590-86-3	40
5	Cyclopropyl carbinol	72	C4H8O	002516-33-8	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011922\
Data File : VU046797.D
Acq On : 19 Jan 2022 14:36
Operator : SY/MD
Sample : N1194-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXX1

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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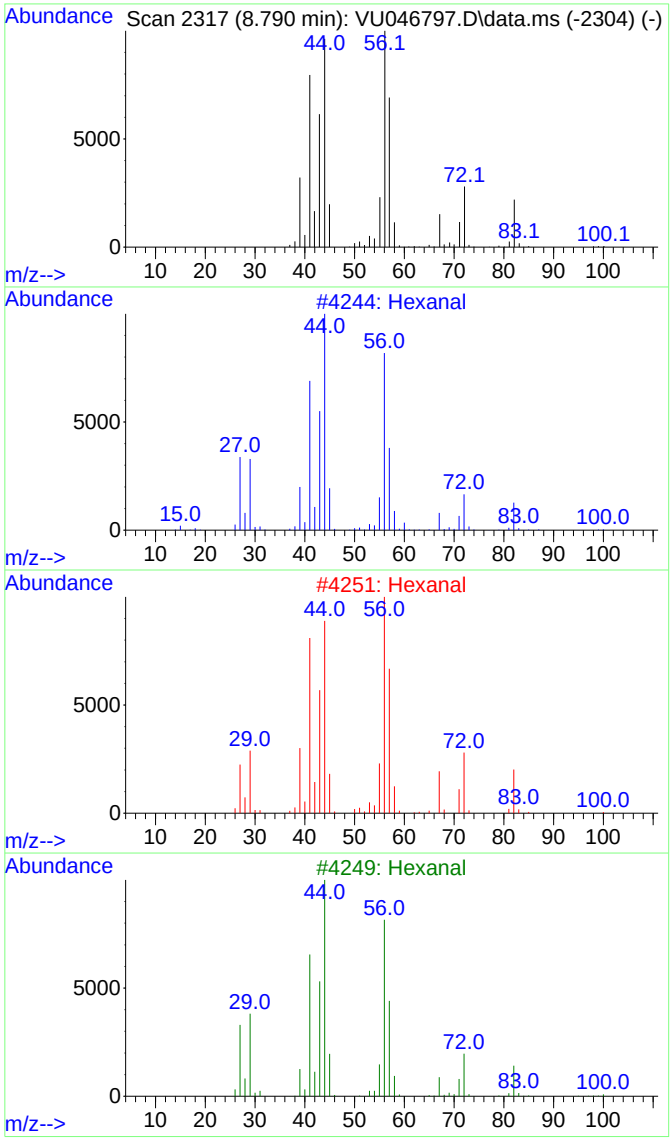
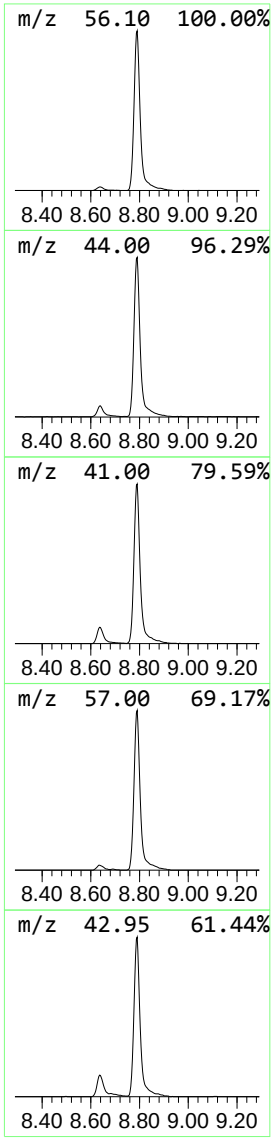
Peak Number 3 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.790	13.90 ug/L	961744	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	94
2	Hexanal	100	C6H12O	000066-25-1	94
3	Hexanal	100	C6H12O	000066-25-1	94
4	Hexanal	100	C6H12O	000066-25-1	90
5	Hexanal	100	C6H12O	000066-25-1	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011922\
Data File : VU046797.D
Acq On : 19 Jan 2022 14:36
Operator : SY/MD
Sample : N1194-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXX1

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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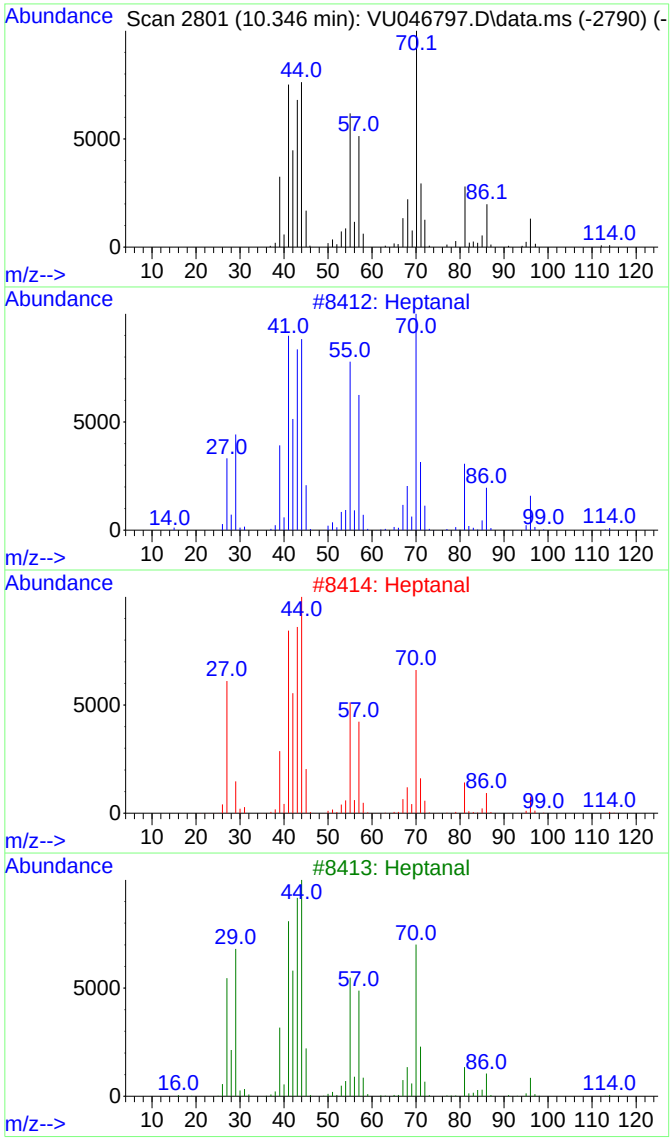
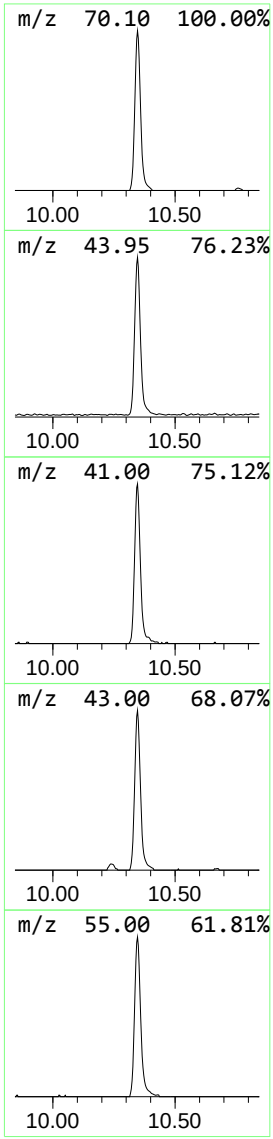
Peak Number 4 Heptanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.346	3.22 ug/L	223005	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal	114	C7H14O	000111-71-7	98
2	Heptanal	114	C7H14O	000111-71-7	95
3	Heptanal	114	C7H14O	000111-71-7	95
4	Heptanal	114	C7H14O	000111-71-7	58
5	Heptanal	114	C7H14O	000111-71-7	46





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011922\
Data File : VU046797.D
Acq On : 19 Jan 2022 14:36
Operator : SY/MD
Sample : N1194-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXX1

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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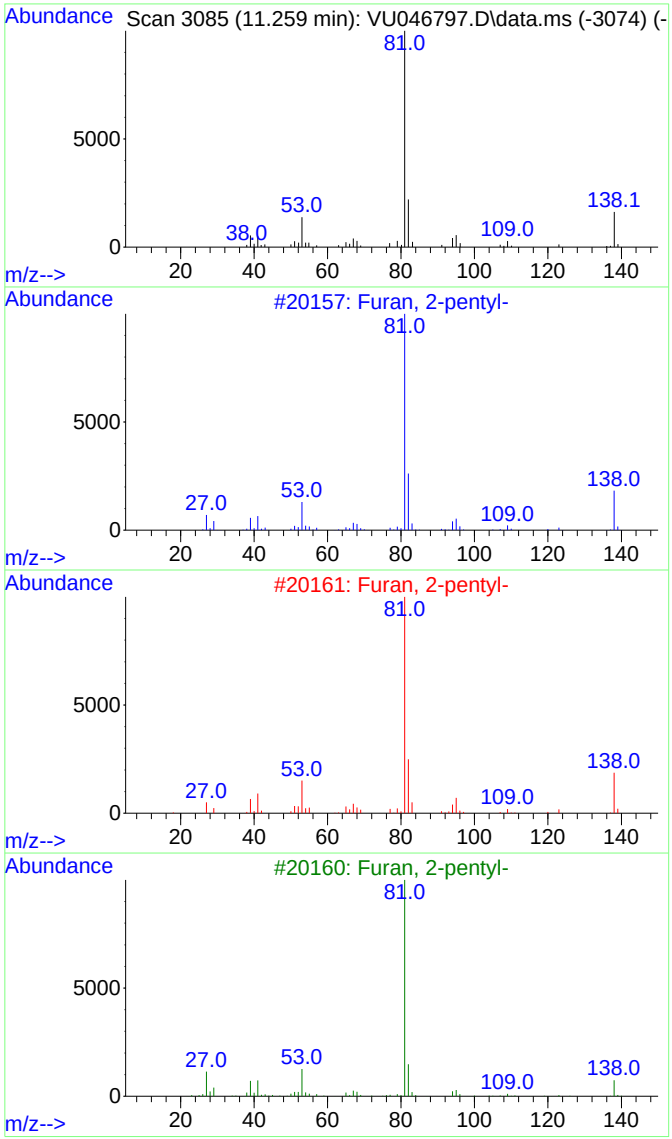
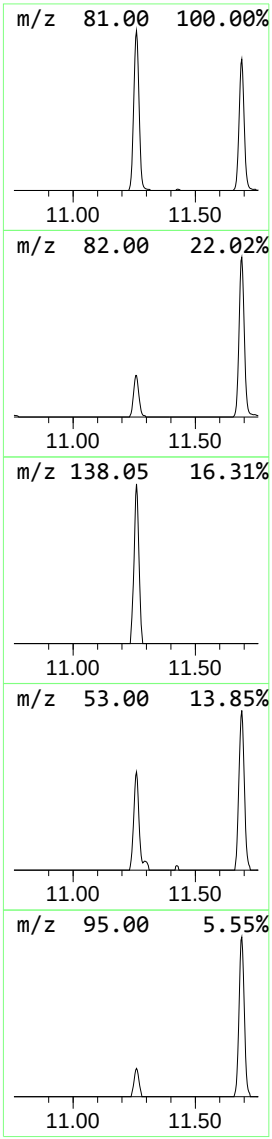
Peak Number 5 Furan, 2-pentyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.259	0.74 ug/L	62031	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, 2-pentyl-	138	C9H14O	003777-69-3	91
2	Furan, 2-pentyl-	138	C9H14O	003777-69-3	91
3	Furan, 2-pentyl-	138	C9H14O	003777-69-3	90
4	2-[(2-Furylmethyl)amino]-2-methy...	169	C9H15NO2	889949-94-4	59
5	Cyclohexene, 4-bromo-	160	C6H9Br	003540-84-9	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011922\
Data File : VU046797.D
Acq On : 19 Jan 2022 14:36
Operator : SY/MD
Sample : N1194-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXX1

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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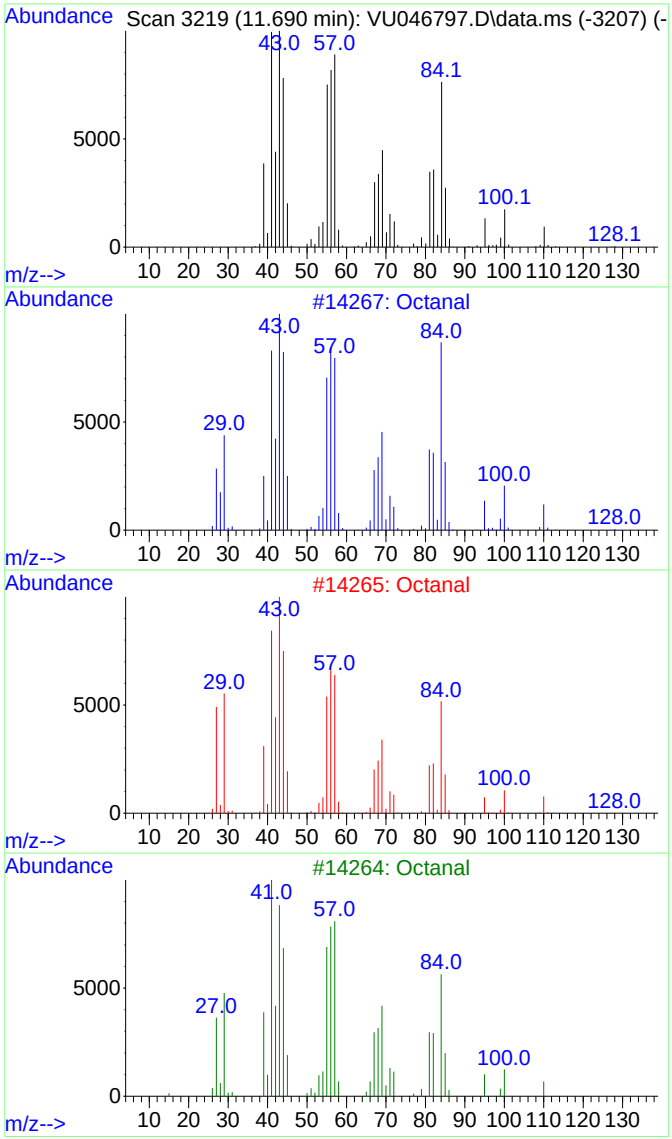
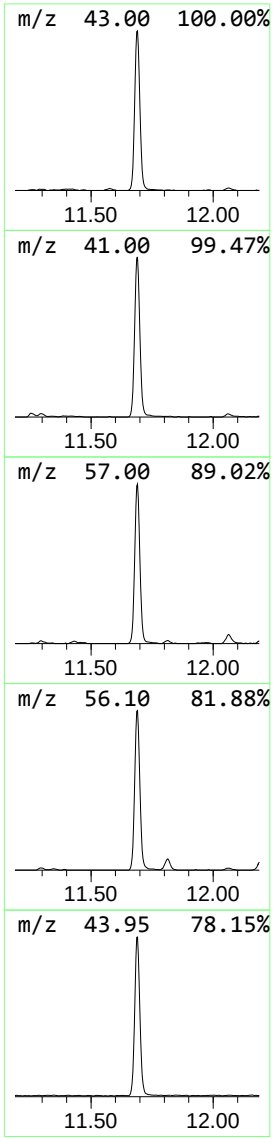
Peak Number 6 Octanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.690	8.48 ug/L	715302	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal	128	C8H16O	000124-13-0	98
2	Octanal	128	C8H16O	000124-13-0	94
3	Octanal	128	C8H16O	000124-13-0	91
4	Octanal	128	C8H16O	000124-13-0	90
5	2-Amino-oxazole	84	C3H4N2O	004570-45-0	64





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Acq On : 19 Jan 2022 14:36
Operator : SY/MD
Sample : N1194-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXX1

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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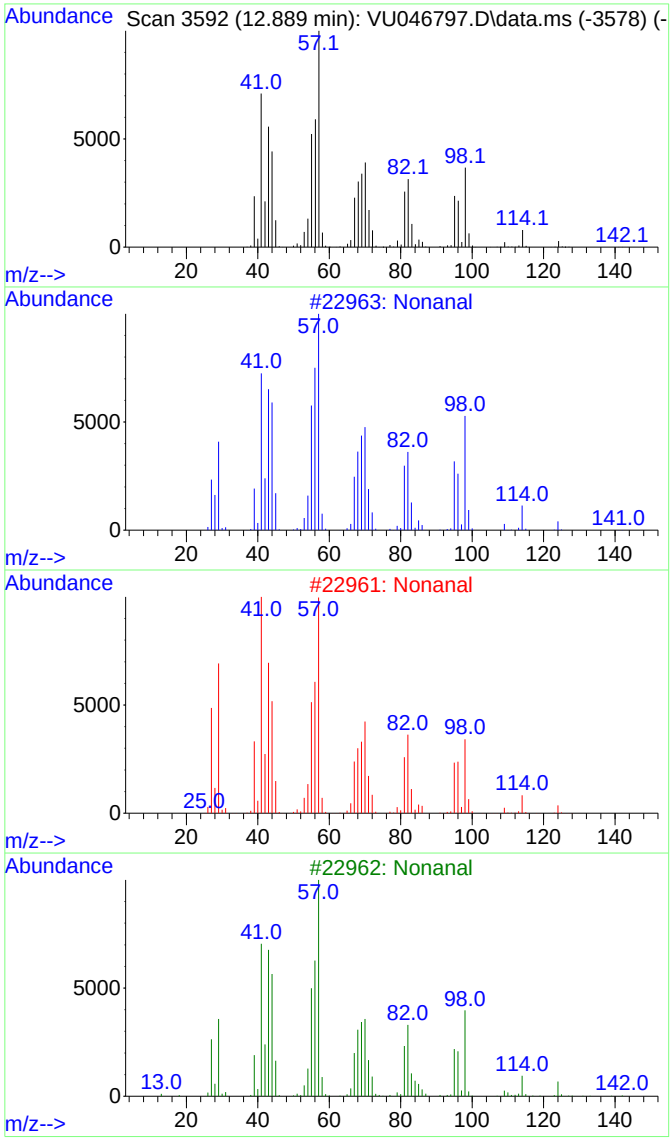
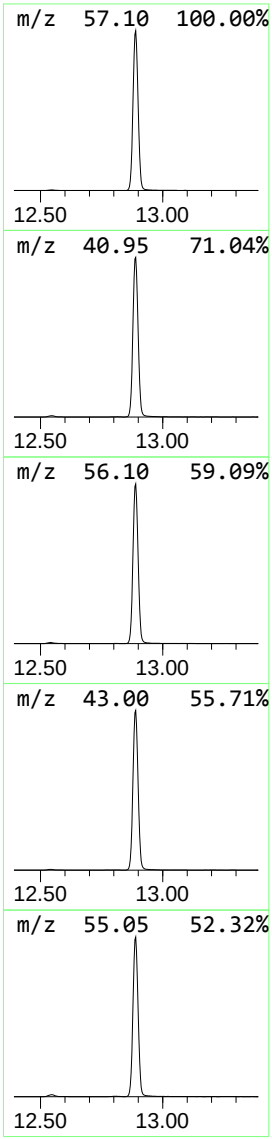
Peak Number 7 Nonanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.890	62.83 ug/L	5297720	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	91
4	Nonanal	142	C9H18O	000124-19-6	83
5	Carbonic acid, heptyl vinyl ester	186	C10H18O3	1010383-25-4	35





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Acq On : 19 Jan 2022 14:36
Operator : SY/MD
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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXX1

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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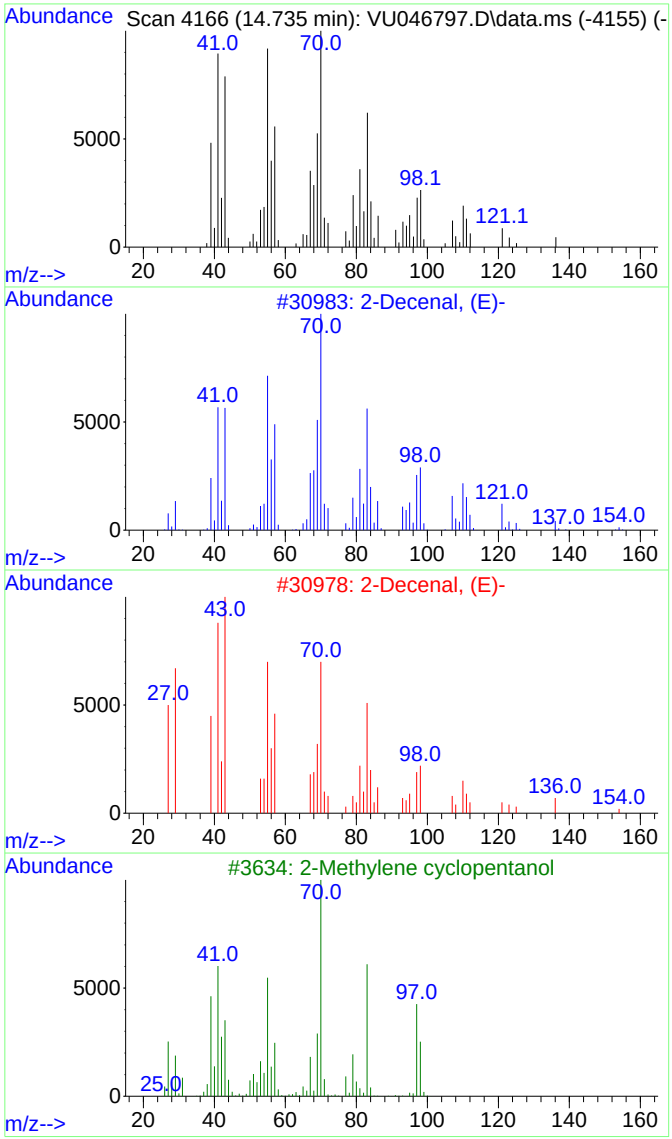
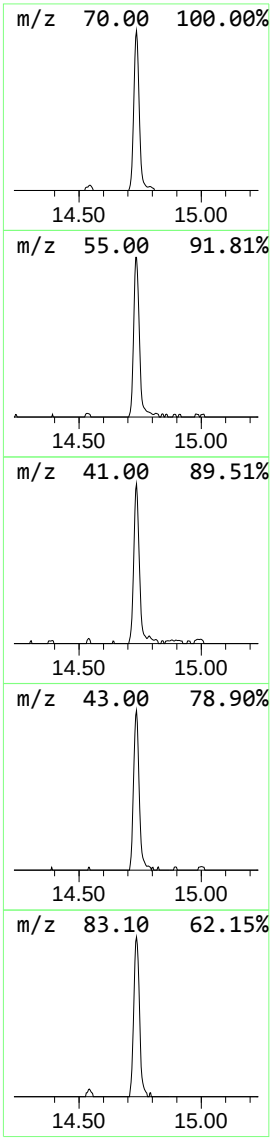
Peak Number 8 2-Decenal, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.735	1.56 ug/L	131305	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Decenal, (E)-	154	C10H18O	003913-81-3	83
2	2-Decenal, (E)-	154	C10H18O	003913-81-3	59
3	2-Methylene cyclopentanol	98	C6H10O	020461-31-8	55
4	Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	46
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011922\
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ClientSampleId :
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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
Pentanal	6.883	1.2	ug/L	58739	1	6.253	251715	5.0
Hexanal	8.790	13.9	ug/L	961744	2	9.420	345924	5.0
Heptanal	10.346	3.2	ug/L	223005	2	9.420	345924	5.0
Furan, 2-pentyl-	11.259	0.7	ug/L	62031	3	11.812	421574	5.0
Octanal	11.690	8.5	ug/L	715302	3	11.812	421574	5.0
Nonanal	12.890	62.8	ug/L	5297720	3	11.812	421574	5.0
2-Decenal, (E)-	14.735	1.6	ug/L	131305	3	11.812	421574	5.0