LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020322\
Data File : VU047028.D
Acq On : 03 Feb 2022 17:50
Operator : SY/MD
Sample : N1348-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXY8

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: VU047028.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.363	3	7	12	rVB2	5131	4590	1.10%	0.100%
2	1.446	27	33	39	rBV	7583	7670	1.84%	0.167%
3	1.601	71	81	100	rVB	54491	68058	16.29%	1.485%
4	1.697	104	111	121	rBV	4621	7241	1.73%	0.158%
5	1.916	171	179	199	rBV	44193	60421	14.46%	1.319%
6	2.144	240	250	260	rVV	8584	13368	3.20%	0.292%
7	2.575	368	384	400	rBV3	109084	218311	52.24%	4.764%
8	3.874	771	788	812	rBV	55142	131321	31.43%	2.866%
9	4.465	960	972	983	rBV5	2152	5777	1.38%	0.126%
10	4.668	1014	1035	1060	rBV3	66823	240908	57.65%	5.257%
11	5.067	1144	1159	1181	rBV2	78901	193354	46.27%	4.220%
12	5.321	1226	1238	1251	rVB3	5937	12941	3.10%	0.282%
13	5.729	1342	1365	1382	rBV2	139975	364893	87.32%	7.963%
14	6.253	1512	1528	1550	rBV	118443	229612	54.95%	5.011%
15	6.546	1602	1619	1635	rBV2	38881	72900	17.45%	1.591%
16	6.694	1652	1665	1684	rBV2	90674	176936	42.34%	3.861%
17	6.880	1712	1723	1744	rBV4	15774	34452	8.24%	0.752%
18	7.568	1923	1937	1959	rVB2	39976	72006	17.23%	1.571%
19	7.903	2023	2041	2060	rBV	139386	261012	62.46%	5.696%
20	8.182	2115	2128	2140	rBV2	24536	41546	9.94%	0.907%
21	8.555	2233	2244	2258	rBV2	41258	71158	17.03%	1.553%
22	8.639	2258	2270	2303	rVV	203812	417877	100.00%	9.119%
23	8.790	2303	2317	2339	rBV	119143	219306	52.48%	4.786%
24	9.420	2499	2513	2533	rBV	197022	349454	83.63%	7.626%
25	10.343	2790	2800	2819	rBV2	36724	62567	14.97%	1.365%
26	10.758	2918	2929	2946	rVB	77066	123410	29.53%	2.693%
27	10.893	2964	2971	2980	rVB2	3543	4752	1.14%	0.104%
28	11.259	3077	3085	3091	rBV	4722	6931	1.66%	0.151%
29	11.295	3091	3096	3105	rVB3	5178	7250	1.73%	0.158%
30	11.388	3117	3125	3133	rBV5	3221	5096	1.22%	0.111%
31	11.687	3208	3218	3236	rBV2	69321	107284	25.67%	2.341%
32	11.812	3243	3257	3277	rBV	227751	362683	86.79%	7.915%
33	12.060	3324	3334	3353	rVB6	3516	7121	1.70%	0.155%
34	12.195	3363	3376	3389	rBV	152633	249437	59.69%	5.444%
35	12.546	3475	3485	3496	rBV5	10617	19284	4.61%	0.421%
36	12.771	3547	3555	3563	rBV2	2961	4481	1.07%	0.098%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020322\
Data File : VU047028.D
Acq On : 03 Feb 2022 17:50
Operator : SY/MD
Sample : N1348-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXY8

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

37	12.886	3580	3591	3612	rBV	179422	278784	66.71%	6.084%
38	13.684	3833	3839	3851	rVB5	4296	6785	1.62%	0.148%
39	14.735	4154	4166	4179	rBV3	32470	51959	12.43%	1.134%
40	15.709	4460	4469	4479	rVB5	6551	9305	2.23%	0.203%

Sum of corrected areas: 4582241

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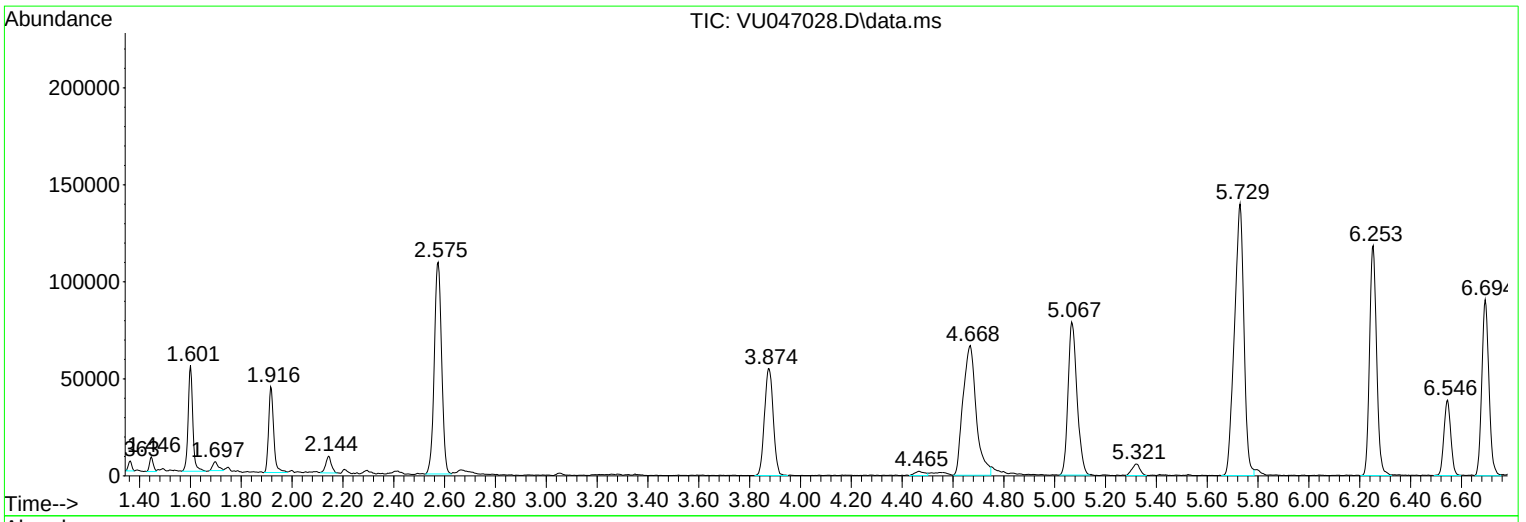
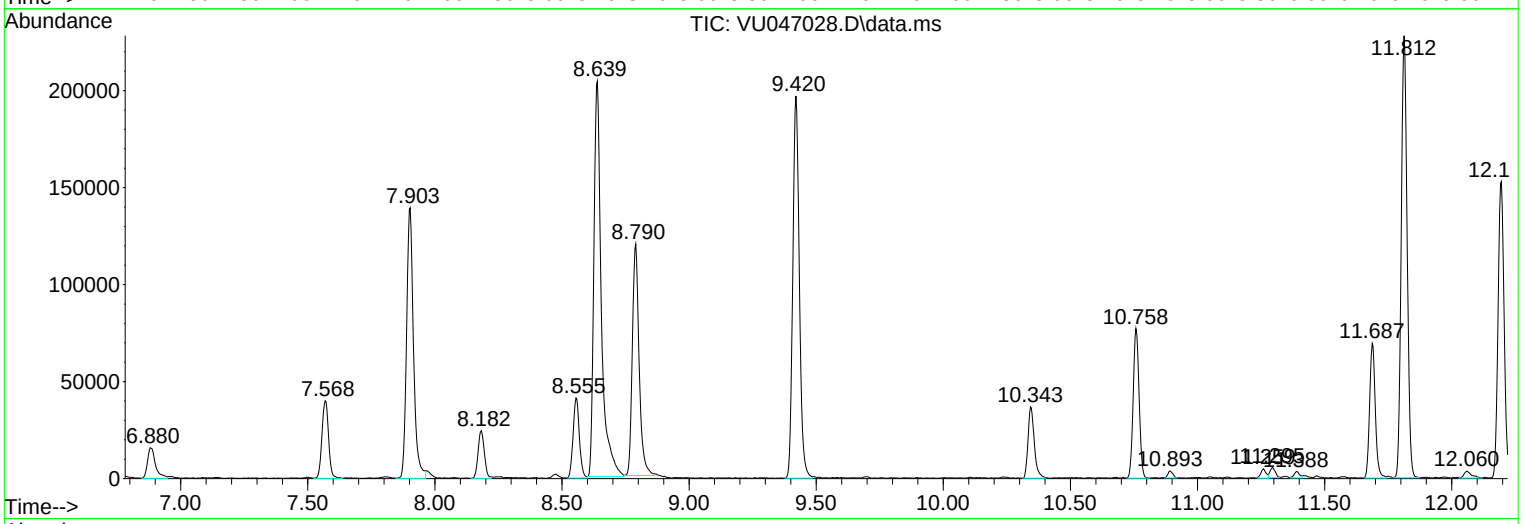
Acq On : 03 Feb 2022 17:50
Operator : SY/MD
Sample : N1348-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

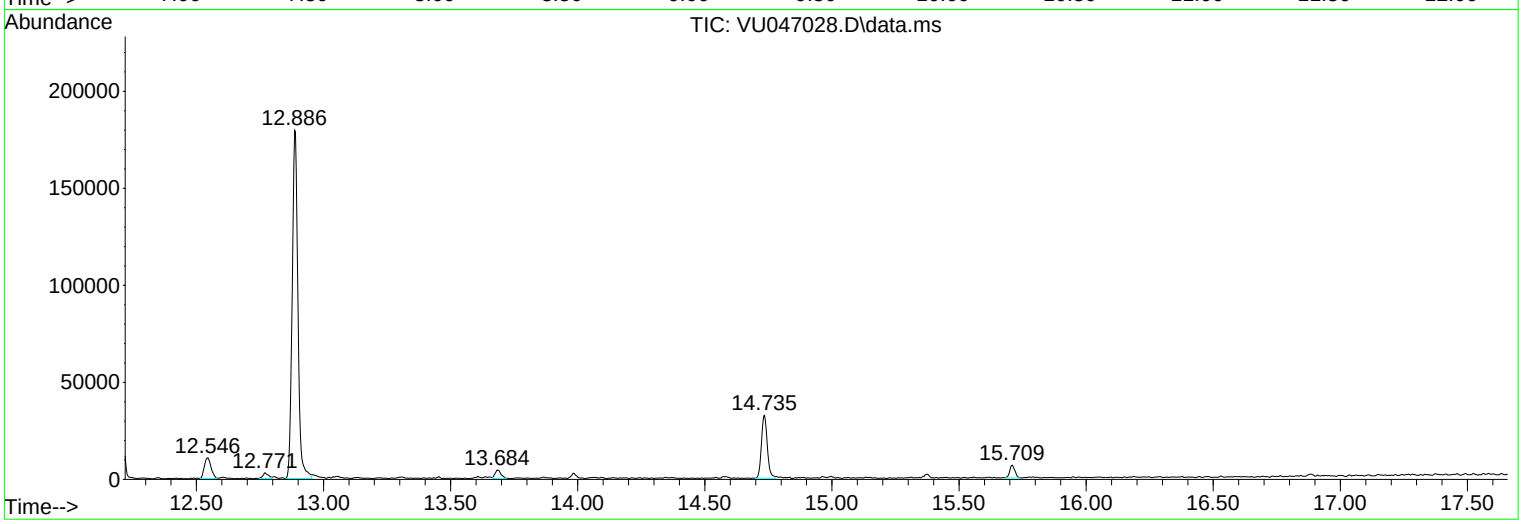
Instrument :
MSVOA_U
ClientSampleId :
BFXY8

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\VU020322\
Data File : VU047028.D
Acq On : 03 Feb 2022 17:50
Operator : SY/MD
Sample : N1348-05
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXY8

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

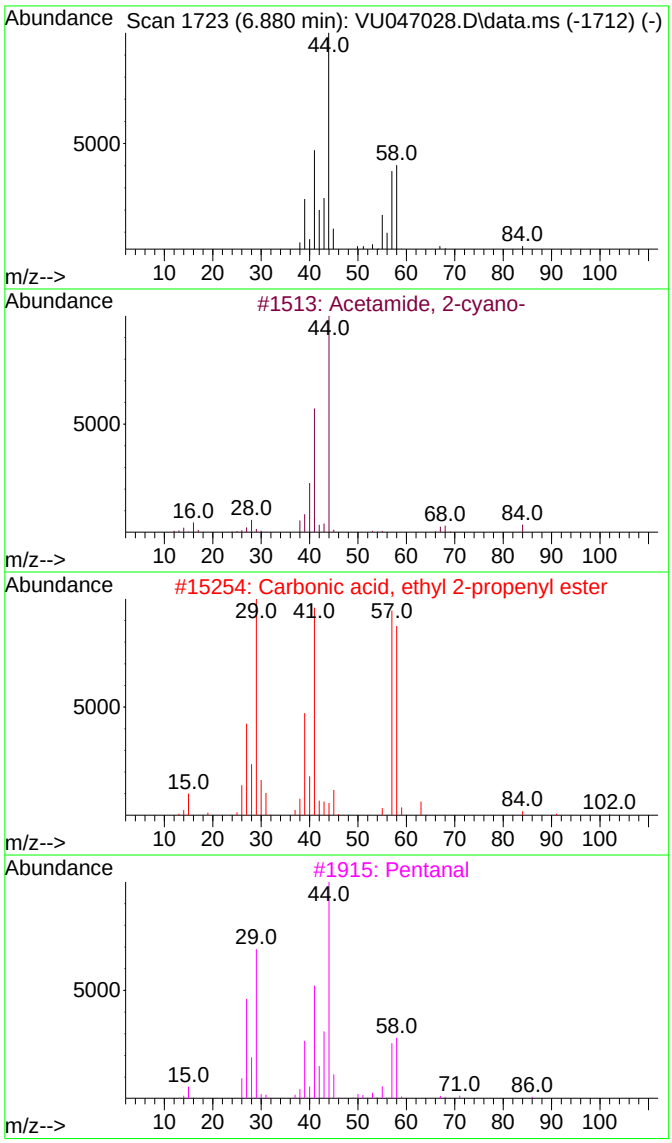
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

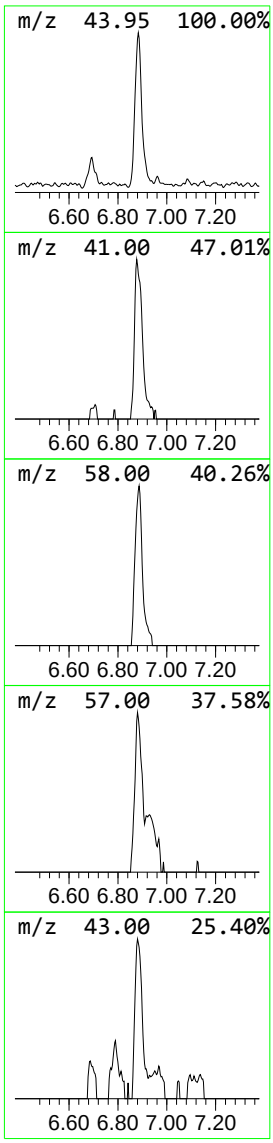
****

Peak Number 1 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.880	0.75 ug/L	34452	1,4-Difluorobenzene	6.253

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, 2-cyano-	84	C3H4N2O	000107-91-5	23
2	Carbonic acid, ethyl 2-propenyl ...	130	C6H10O3	001469-70-1	9
3	Pentanal	86	C5H10O	000110-62-3	9
4	Methylpent-4-enylamine	99	C6H13N	005831-72-1	9
5	Pentanal	86	C5H10O	000110-62-3	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020322\
Data File : VU047028.D
Acq On : 03 Feb 2022 17:50
Operator : SY/MD
Sample : N1348-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXY8

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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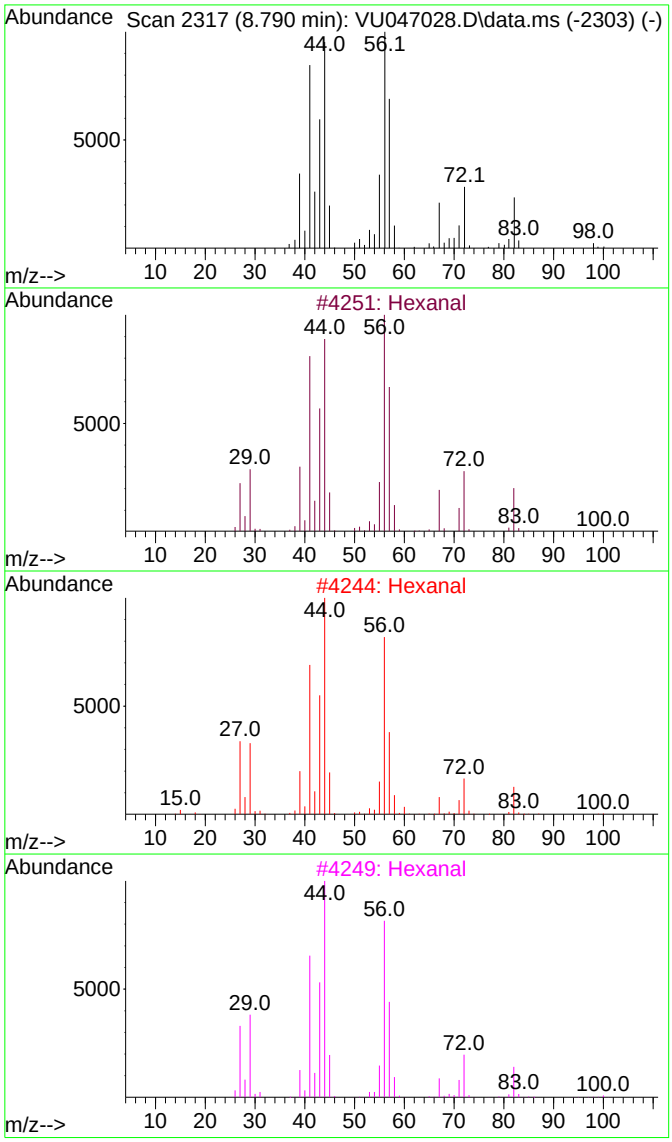
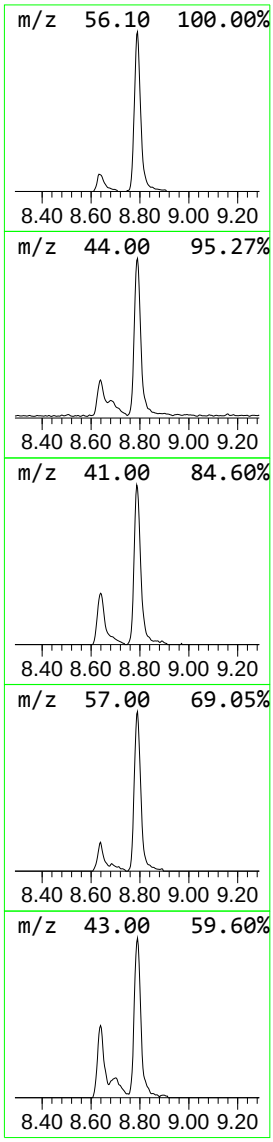
Peak Number 3 Hexanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.790	3.14 ug/L	219306	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	95
2	Hexanal	100	C6H12O	000066-25-1	87
3	Hexanal	100	C6H12O	000066-25-1	86
4	Hexanal	100	C6H12O	000066-25-1	86
5	Hexanal	100	C6H12O	000066-25-1	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020322\
Data File : VU047028.D
Acq On : 03 Feb 2022 17:50
Operator : SY/MD
Sample : N1348-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXY8

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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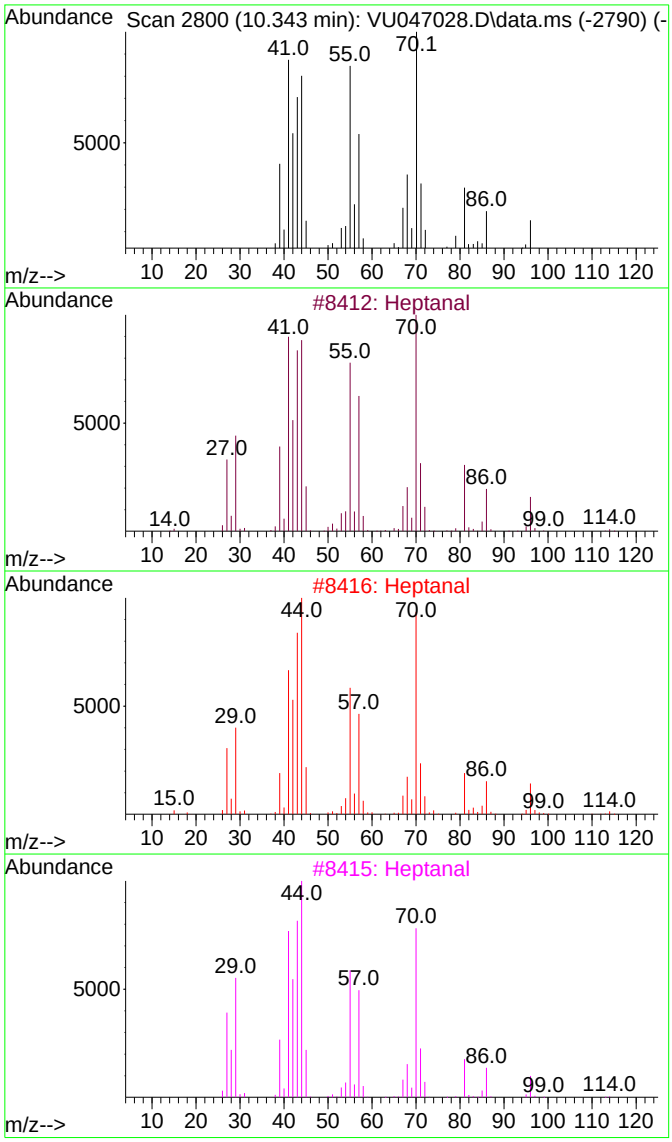
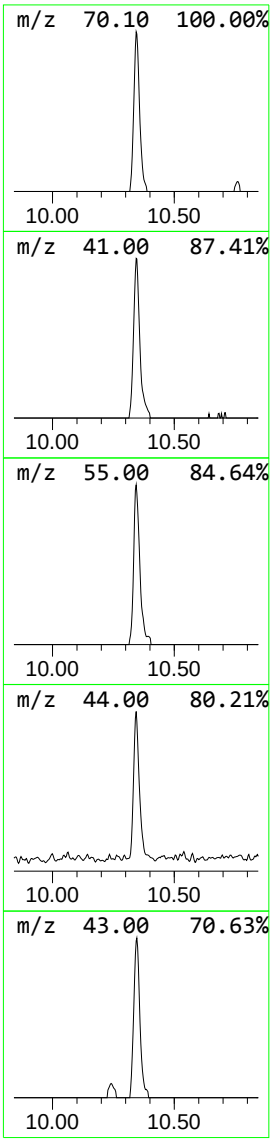
Peak Number 4 Heptanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.343	0.90 ug/L	62567	Chlorobenzene-d5	9.420

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal	114	C7H14O	000111-71-7	80
2	Heptanal	114	C7H14O	000111-71-7	50
3	Heptanal	114	C7H14O	000111-71-7	45
4	Heptanal	114	C7H14O	000111-71-7	45
5	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020322\
Data File : VU047028.D
Acq On : 03 Feb 2022 17:50
Operator : SY/MD
Sample : N1348-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXY8

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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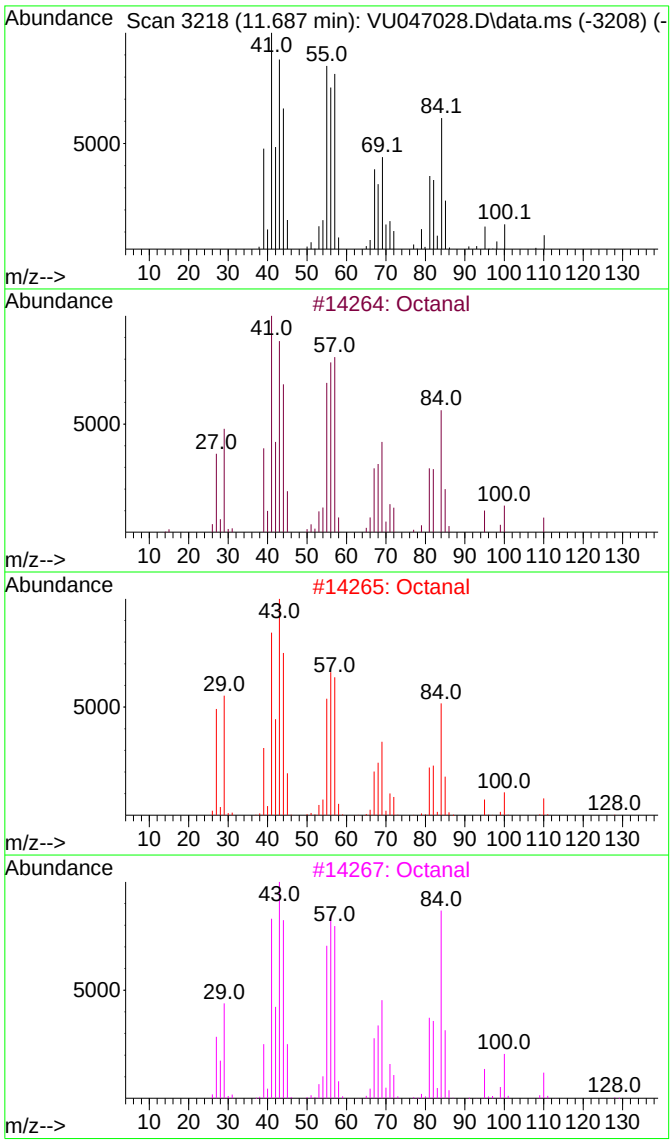
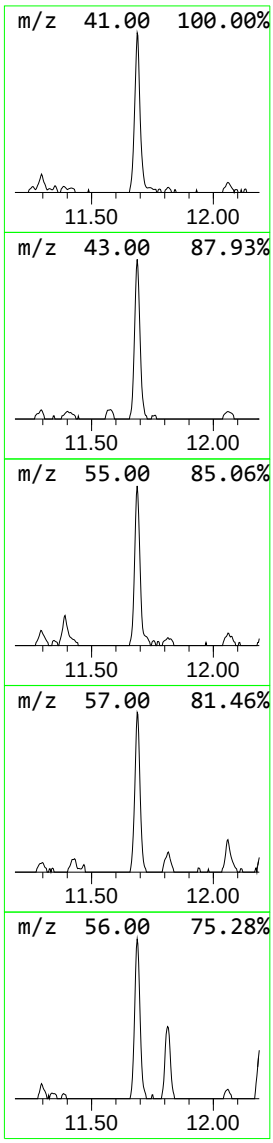
Peak Number 5 Octanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.687	1.48 ug/L	107284	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	72
3	Octanal	128	C8H16O	000124-13-0	72
4	Octanal	128	C8H16O	000124-13-0	64
5	1-Pentene, 3-methyl-	84	C6H12	000760-20-3	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020322\
Data File : VU047028.D
Acq On : 03 Feb 2022 17:50
Operator : SY/MD
Sample : N1348-05
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXY8

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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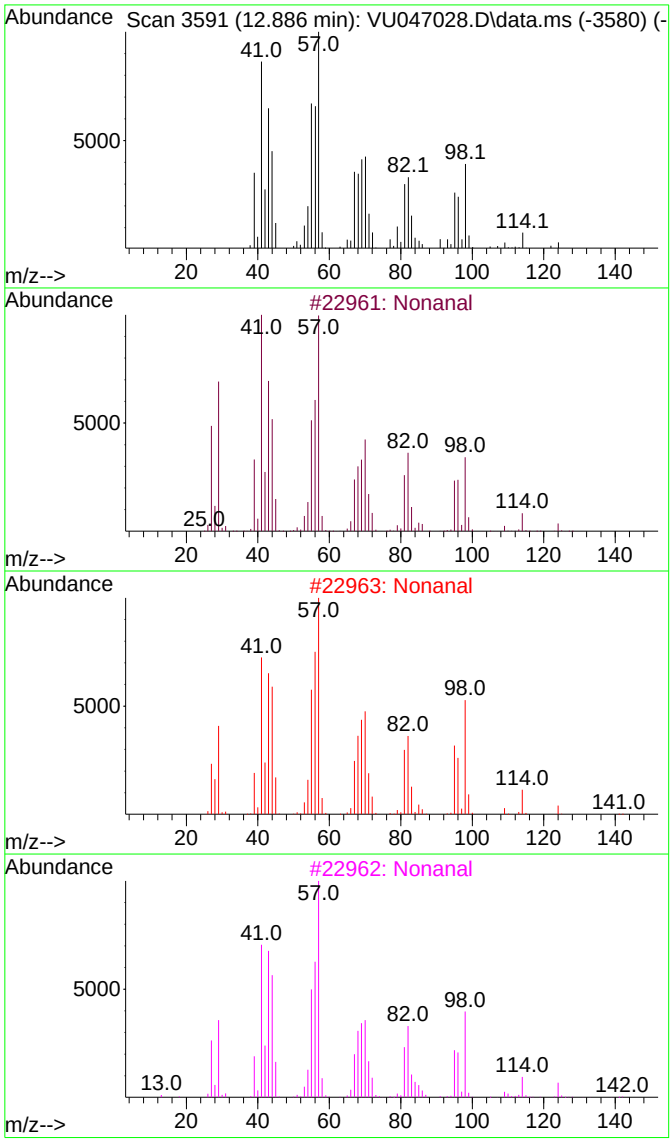
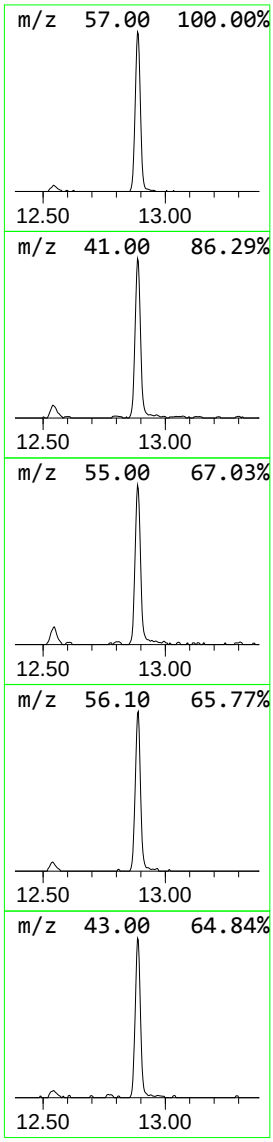
Peak Number 6 Nonanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.886	3.84 ug/L	278784	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	Cycloheptane	98	C7H14	000291-64-5	43
5	Cyclohexanol, 2-methyl-, cis-	114	C7H14O	007443-70-1	30





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Data File : VU047028.D
Acq On : 03 Feb 2022 17:50
Operator : SY/MD
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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFXY8

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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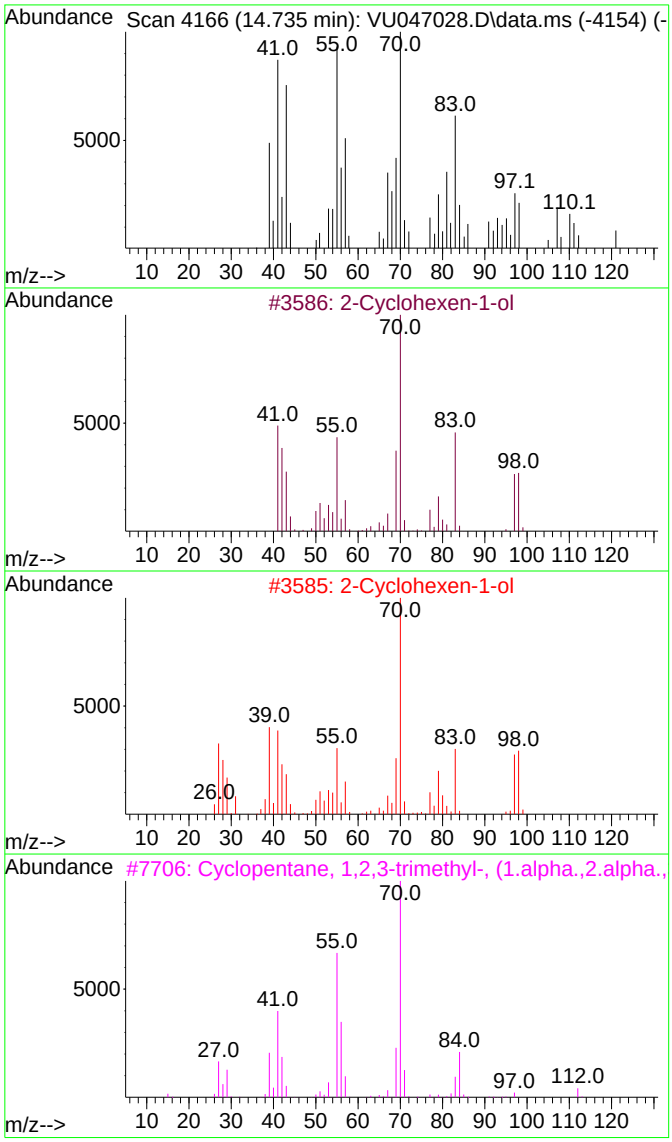
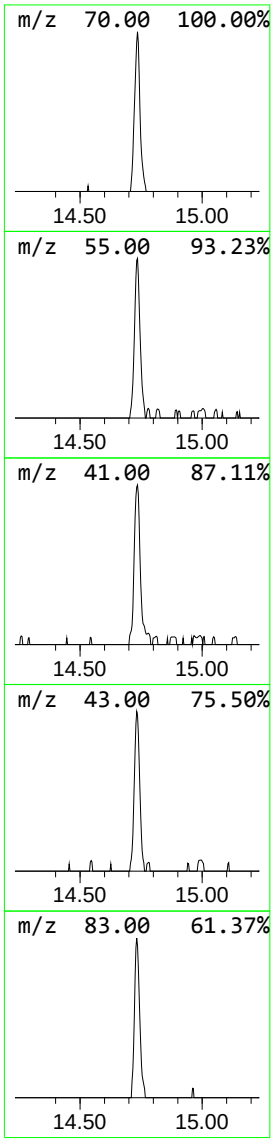
Peak Number 7 2-Cyclohexen-1-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.735	0.72 ug/L	51959	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	53
2	2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	49
3	Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	38
4	Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	002613-69-6	30
5	2-Heptenal, (Z)-	112	C7H12O	057266-86-1	30





Tentatively Identified Compound (LSC) summary

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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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown-01	6.880	0.8	ug/L	34452	1	6.253	229612	5.0
Hexanal	8.790	3.1	ug/L	219306	2	9.420	349454	5.0
Heptanal	10.343	0.9	ug/L	62567	2	9.420	349454	5.0
Octanal	11.687	1.5	ug/L	107284	3	11.812	362683	5.0
Nonanal	12.886	3.8	ug/L	278784	3	11.812	362683	5.0
2-Cyclohexen-1-ol	14.735	0.7	ug/L	51959	3	11.812	362683	5.0