LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072424\
Data File : VU060165.D
Acq On : 24 Jul 2024 19:51
Operator : MD/SY
Sample : P3344-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB71

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\SFAMUTR071824WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU060165.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.596	84	95	111	rBV	134150	177951	10.07%	1.391%
2	1.686	113	123	160	rBV	870721	1368151	77.41%	10.696%
3	1.911	184	193	208	rBV	110418	150274	8.50%	1.175%
4	2.560	379	395	407	rBV2	206967	360808	20.41%	2.821%
5	2.640	407	420	474	rVV	564249	1767437	100.00%	13.817%
6	3.229	574	603	604	rBV3	23901	73286	4.15%	0.573%
7	4.435	959	978	1005	rBV4	115568	330558	18.70%	2.584%
8	4.624	1026	1037	1054	rBV2	151955	436540	24.70%	3.413%
9	5.055	1155	1171	1206	rBV	205454	464981	26.31%	3.635%
10	5.718	1357	1377	1409	rBV2	390984	1024688	57.98%	8.011%
11	6.242	1524	1540	1565	rBV	354831	713204	40.35%	5.576%
12	6.682	1664	1677	1697	rBV2	246380	523587	29.62%	4.093%
13	6.769	1697	1704	1728	rVB	38004	80921	4.58%	0.633%
14	6.875	1728	1737	1748	rBV3	39502	75282	4.26%	0.589%
15	7.123	1800	1814	1819	rBV3	23460	45517	2.58%	0.356%
16	7.560	1938	1950	1974	rBV	108813	193629	10.96%	1.514%
17	7.891	2037	2053	2082	rBV	465810	831492	47.05%	6.500%
18	8.174	2130	2141	2154	rBV2	70469	125524	7.10%	0.981%
19	8.422	2210	2218	2228	rBV2	15344	27076	1.53%	0.212%
20	8.627	2271	2282	2294	rBV	586890	1061205	60.04%	8.296%
21	8.782	2321	2330	2362	rVB2	48469	92192	5.22%	0.721%
22	9.412	2513	2526	2547	rBV	521438	874380	49.47%	6.836%
23	9.647	2589	2599	2609	rBV2	14321	23533	1.33%	0.184%
24	10.232	2769	2781	2798	rBV	92889	159133	9.00%	1.244%
25	10.749	2929	2942	2957	rBV	201046	321800	18.21%	2.516%
26	10.859	2967	2976	2994	rVB3	15834	27179	1.54%	0.212%
27	11.807	3259	3271	3290	rBV	481262	767204	43.41%	5.998%
28	12.187	3377	3389	3408	rBV	431585	693965	39.26%	5.425%

Sum of corrected areas: 12791497

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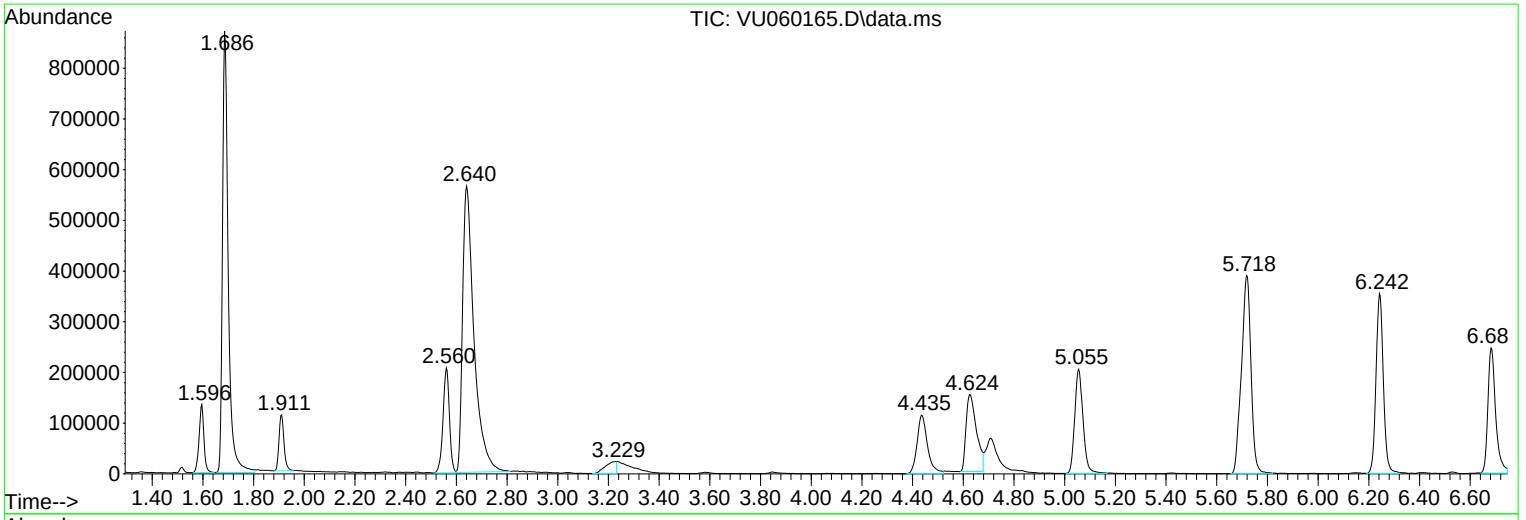
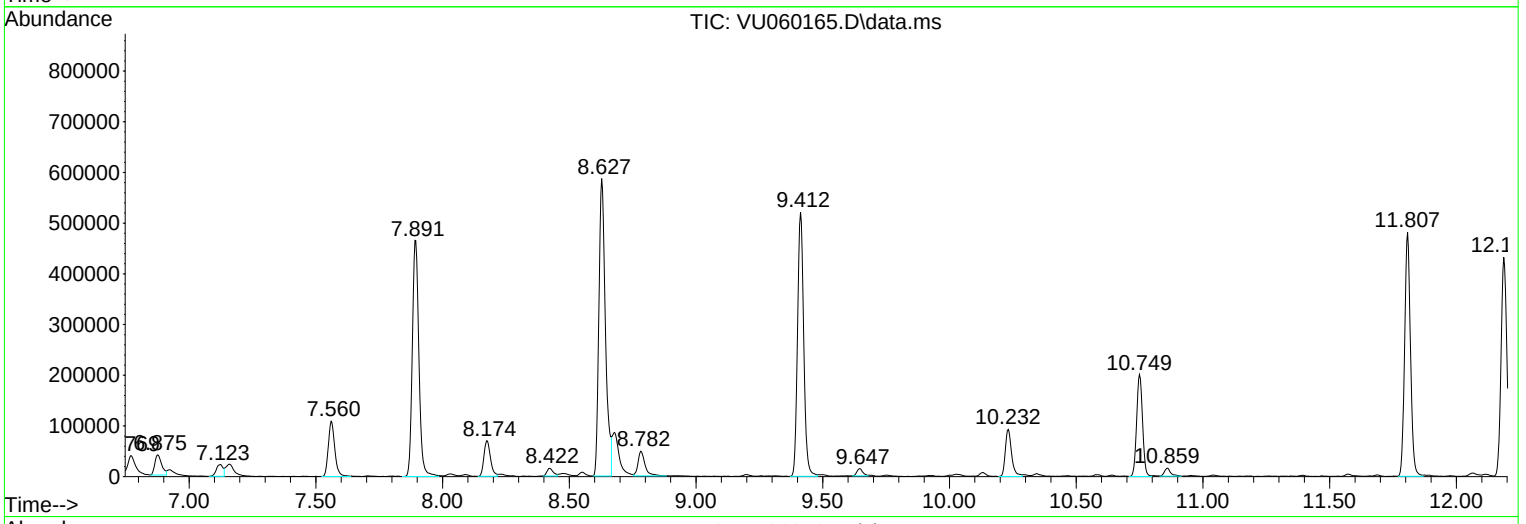
ALS Vial : 19 Sample Multiplier: 1

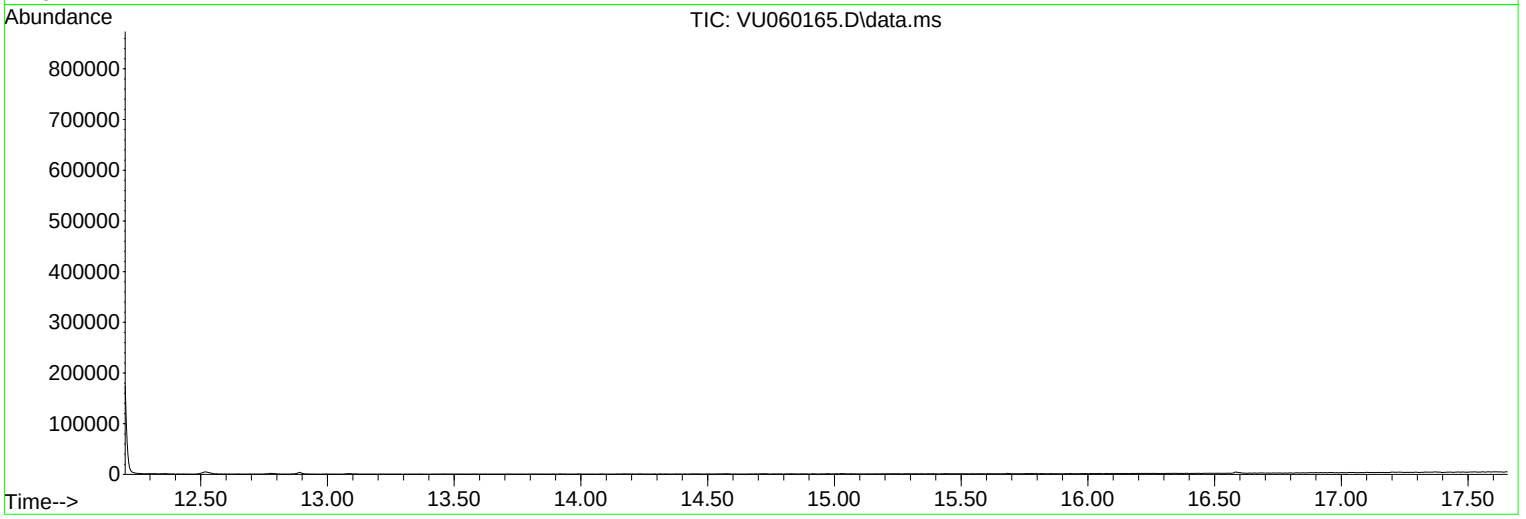
Instrument :
MSVOA_U
ClientSampleId :
BHB71

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR071824WMA.M
Quant Title : TRACE VOA SFAM1.0

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







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Data File : VU060165.D
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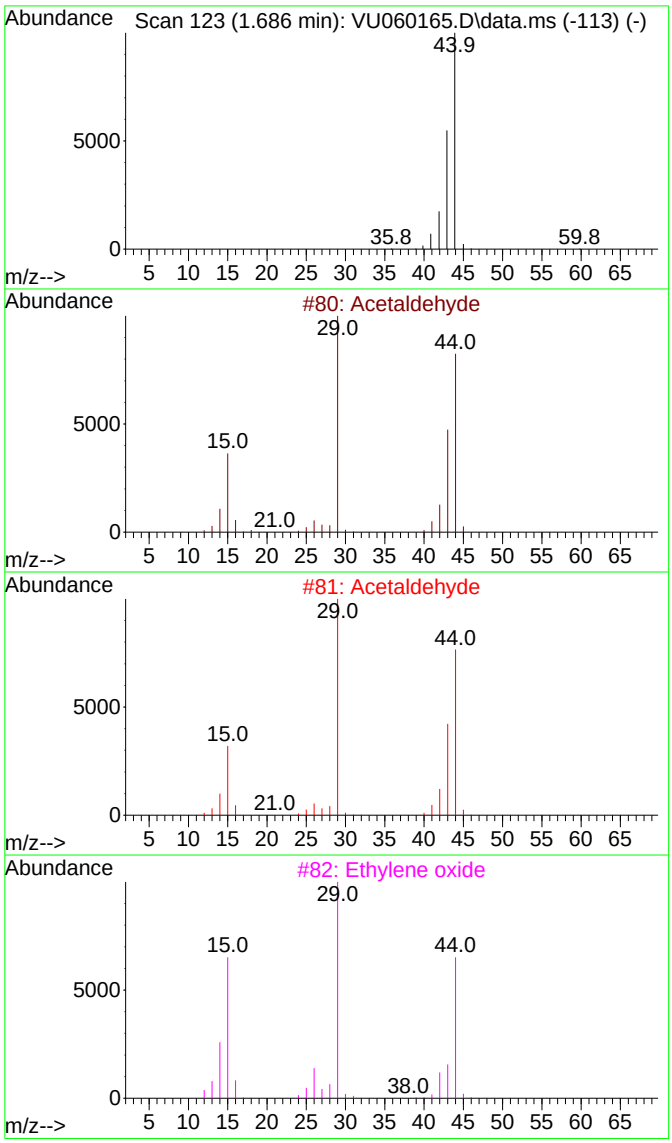
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR071824WMA.M
Quant Title : TRACE VOA SFAM1.0

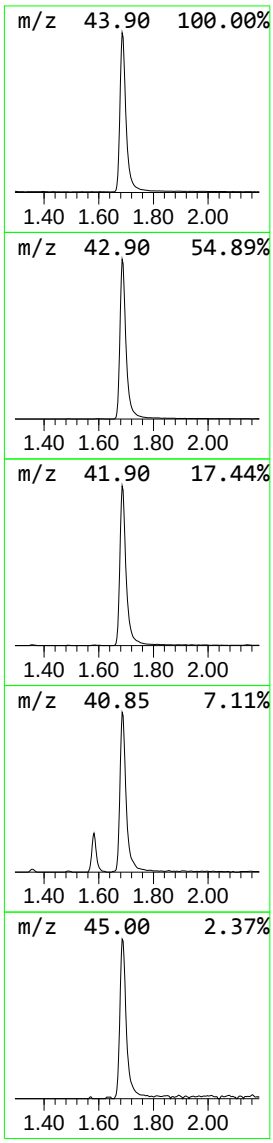
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.686	9.59 ug/L	1368150	1,4-Difluorobenzene	6.242

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	9
2	Acetaldehyde	44	C2H4O	000075-07-0	9
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Ethylene oxide	44	C2H4O	000075-21-8	5
5	Ethylene oxide	44	C2H4O	000075-21-8	5





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Data File : VU060165.D
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Operator : MD/SY
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB71

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR071824WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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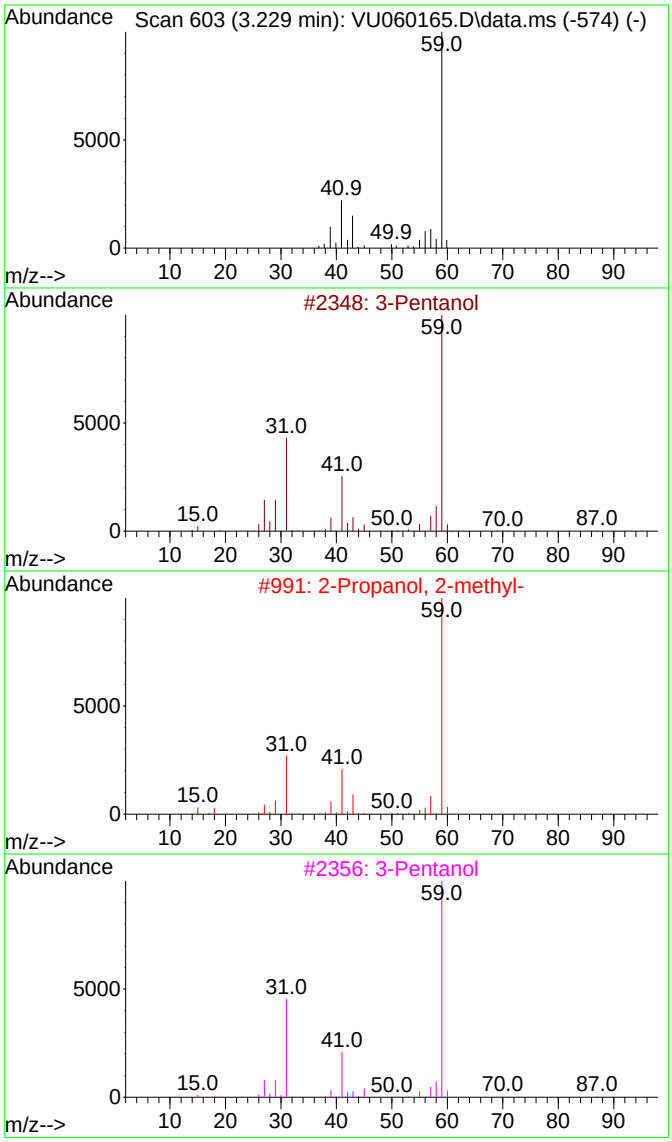
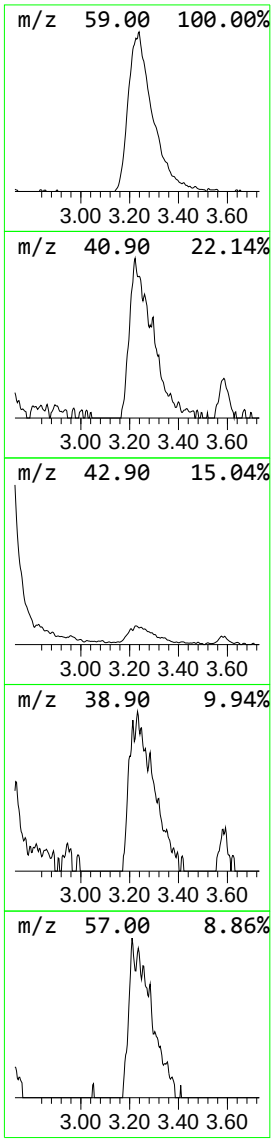
Peak Number 2 unknown-02 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.229	0.51 ug/L	73286	1,4-Difluorobenzene	6.242

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanol	88	C5H12O	000584-02-1	9
2	2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	9
3	3-Pentanol	88	C5H12O	000584-02-1	9
4	3-Pentanol	88	C5H12O	000584-02-1	9
5	3-Pentanol	88	C5H12O	000584-02-1	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072424\
Data File : VU060165.D
Acq On : 24 Jul 2024 19:51
Operator : MD/SY
Sample : P3344-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB71

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR071824WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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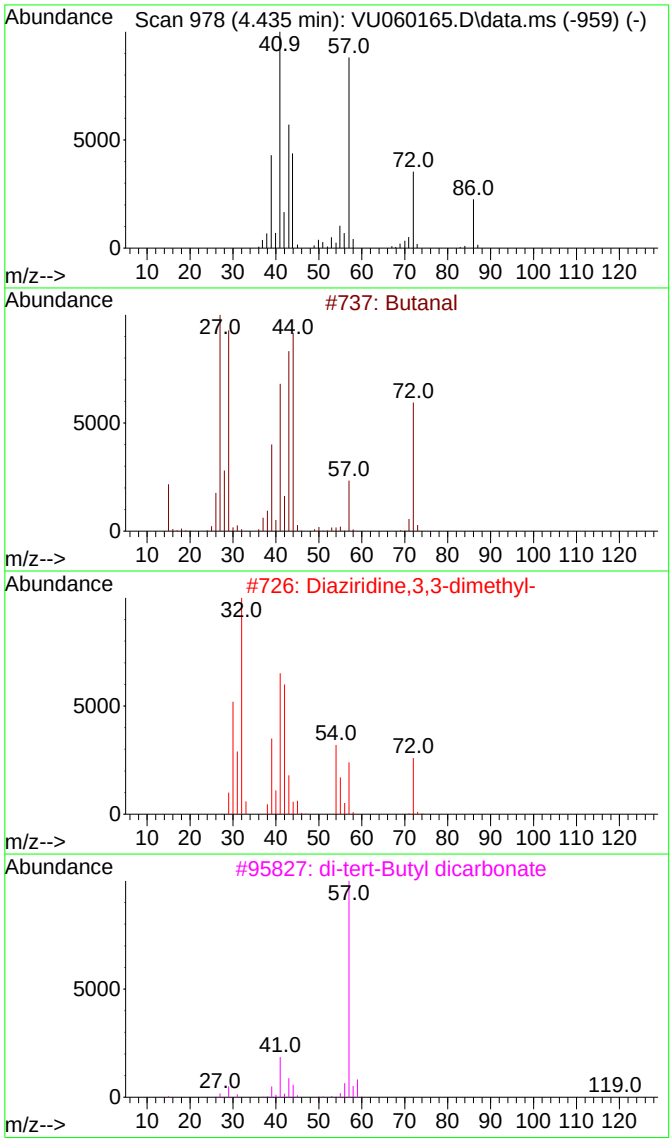
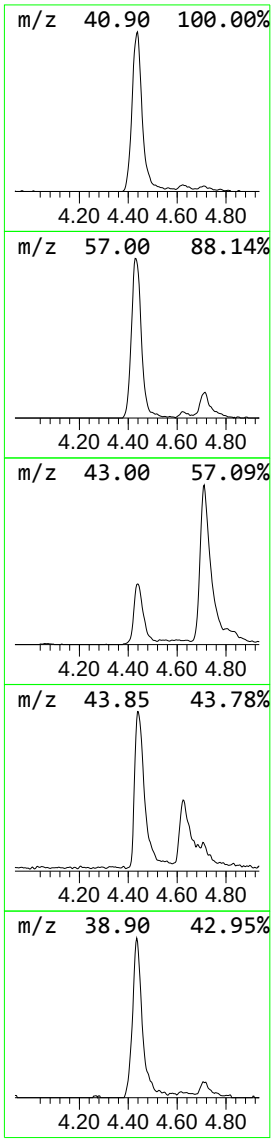
Peak Number 3 unknown-03 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.435	2.32 ug/L	330558	1,4-Difluorobenzene	6.242

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	43
2	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
3	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	32
4	2-Propen-1-ol, 2-methyl-	72	C4H8O	000513-42-8	23
5	2-Buten-1-ol, (E)-	72	C4H8O	000504-61-0	17





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Data File : VU060165.D
Acq On : 24 Jul 2024 19:51
Operator : MD/SY
Sample : P3344-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB71

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR071824WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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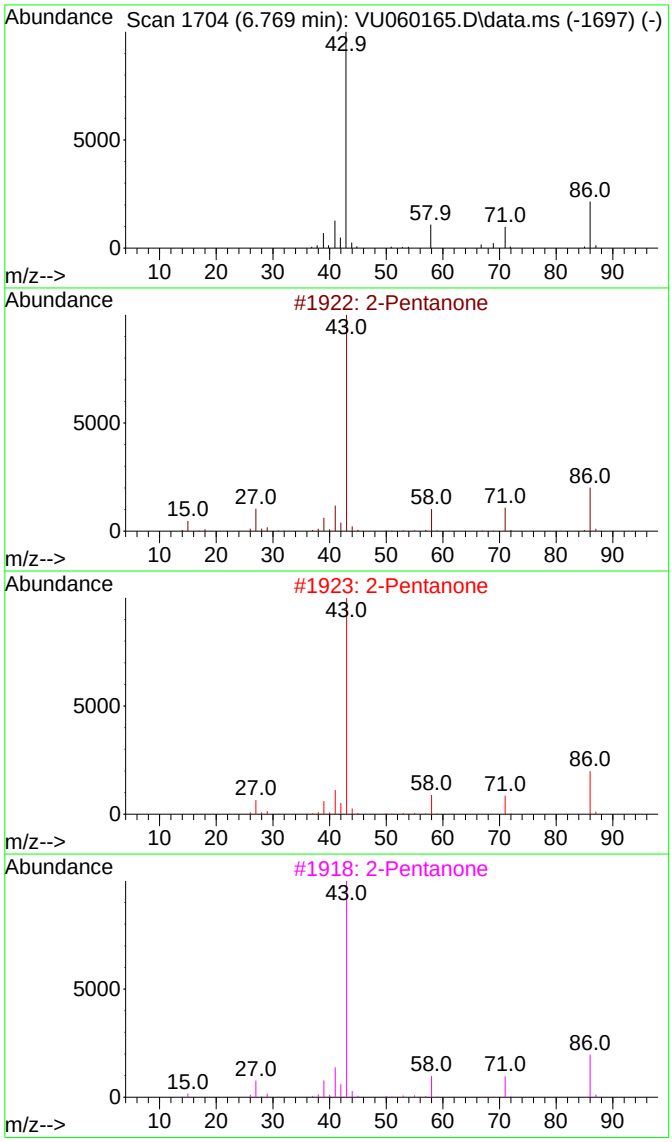
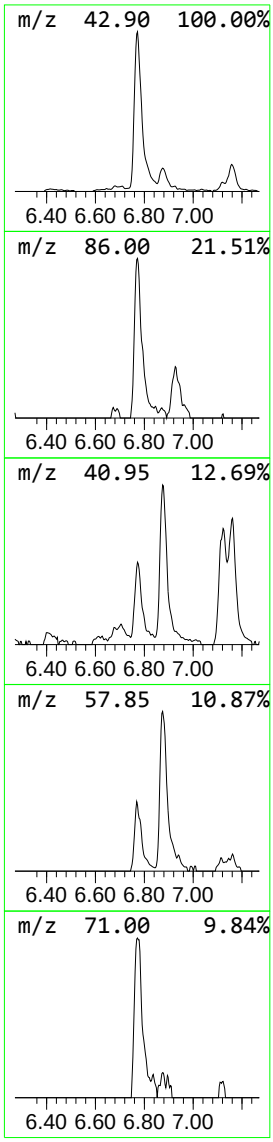
Peak Number 4 2-Pentanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.769	0.57 ug/L	80921	1,4-Difluorobenzene	6.242

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	86
2	2-Pentanone	86	C5H10O	000107-87-9	80
3	2-Pentanone	86	C5H10O	000107-87-9	80
4	2-Pentanone	86	C5H10O	000107-87-9	64
5	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072424\
Data File : VU060165.D
Acq On : 24 Jul 2024 19:51
Operator : MD/SY
Sample : P3344-14
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHB71

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR071824WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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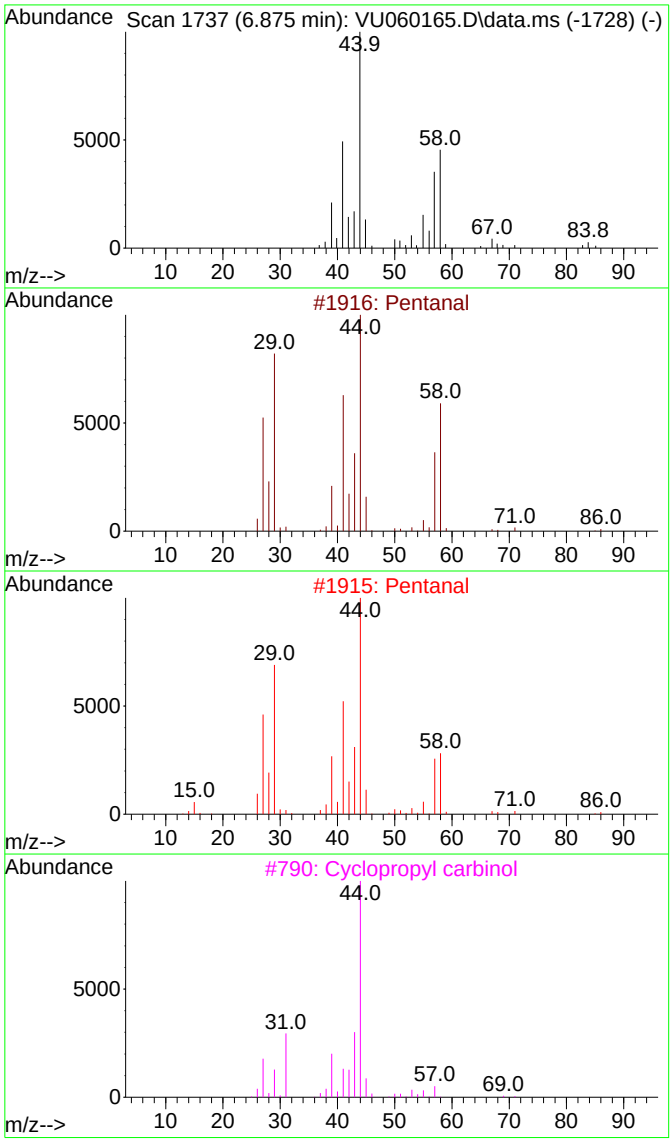
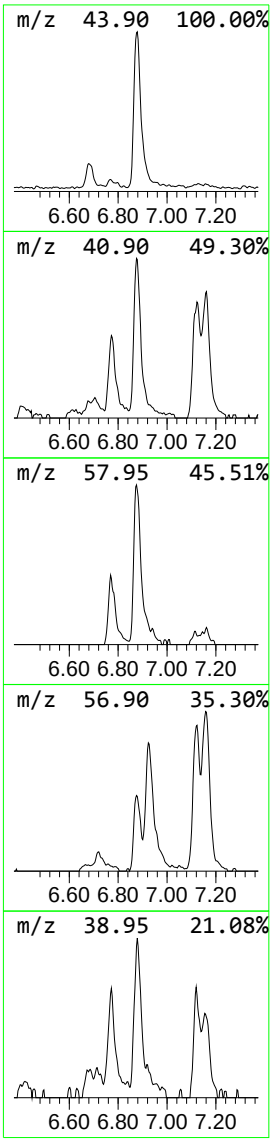
Peak Number 5 Pentanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.875	0.53 ug/L	75282	1,4-Difluorobenzene	6.242

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	Cyclopropyl carbinol	72	C4H8O	002516-33-8	9
4	Cyclopropyl carbinol	72	C4H8O	002516-33-8	9
5	Carbonic acid, ethyl 2-propenyl ...	130	C6H10O3	001469-70-1	9





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR071824WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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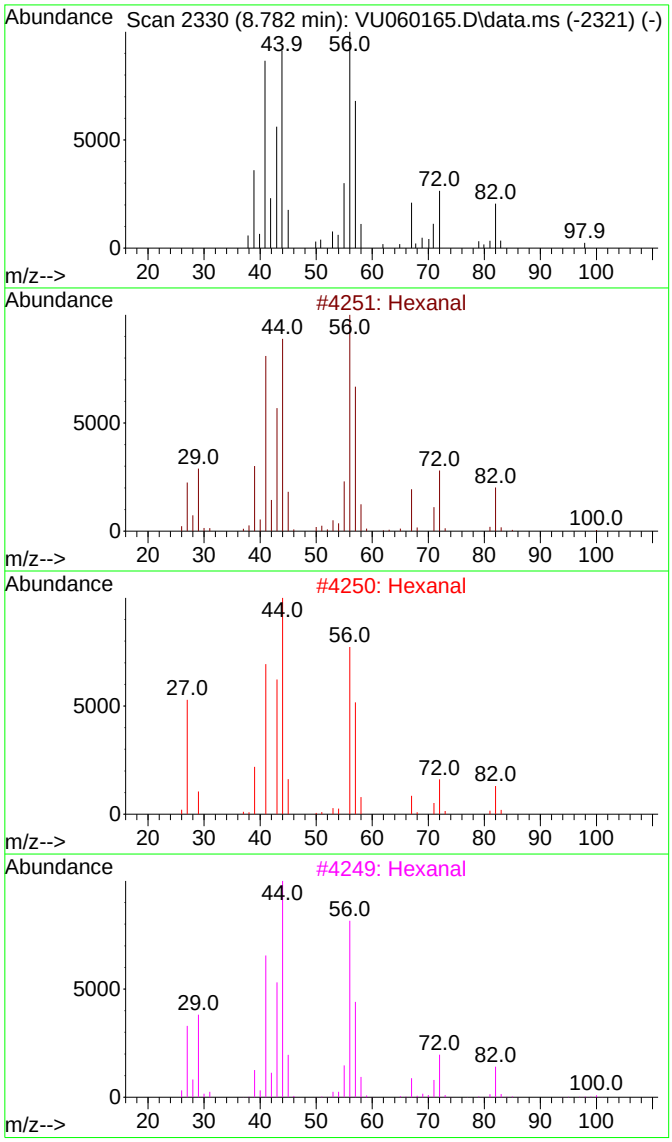
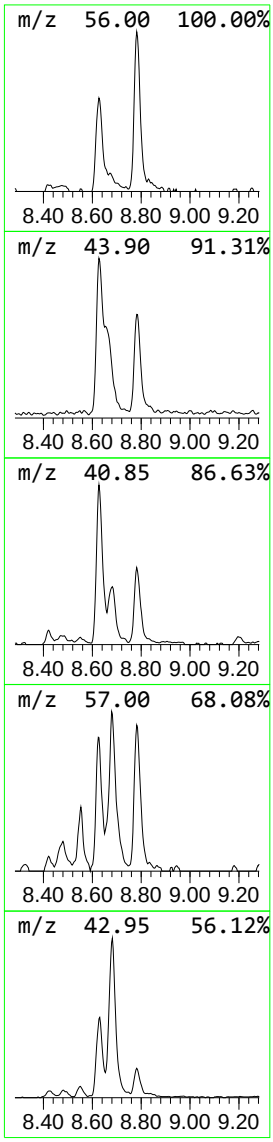
Peak Number 7 Hexanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.782	0.53 ug/L	92192	Chlorobenzene-d5	9.412

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	90
2	Hexanal	100	C6H12O	000066-25-1	86
3	Hexanal	100	C6H12O	000066-25-1	78
4	Hexanal	100	C6H12O	000066-25-1	78
5	Hexanal	100	C6H12O	000066-25-1	64





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MSVOA_U
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR071824WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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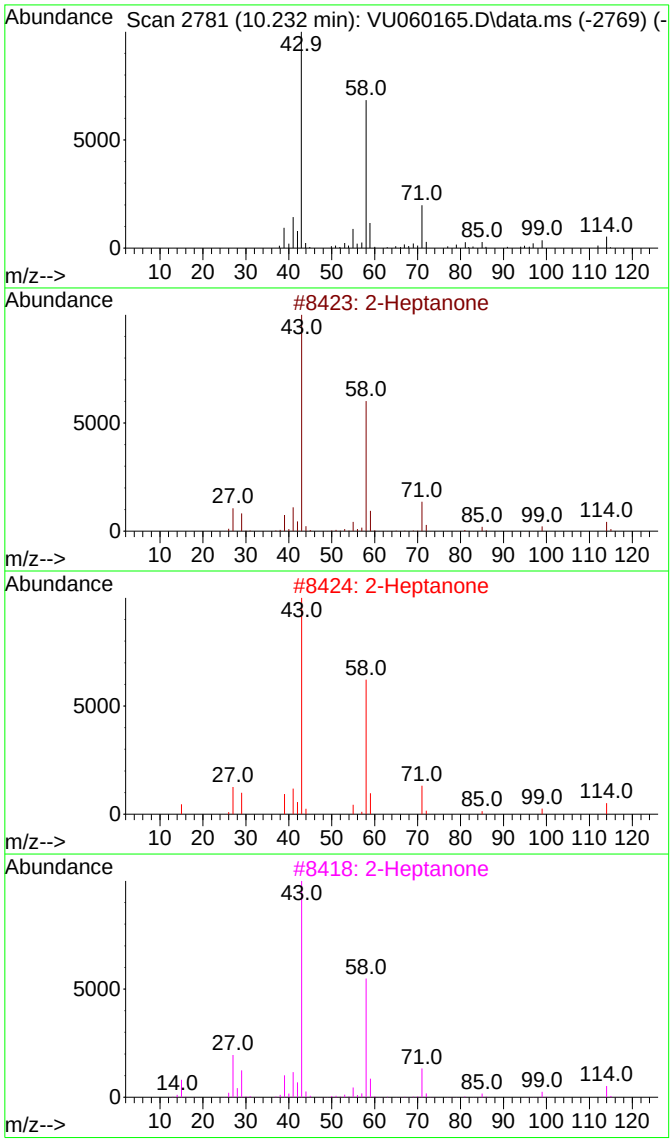
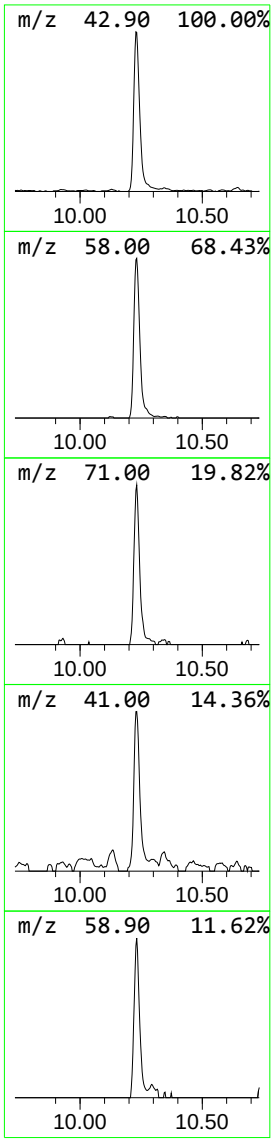
Peak Number 8 2-Heptanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.232	0.91 ug/L	159133	Chlorobenzene-d5	9.412

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone	114	C7H14O	000110-43-0	90
2	2-Heptanone	114	C7H14O	000110-43-0	90
3	2-Heptanone	114	C7H14O	000110-43-0	90
4	2-Heptanone	114	C7H14O	000110-43-0	80
5	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	78





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
unknown-01	1.686	9.6	ug/L	1368150	1	6.242	713204	5.0
unknown-02	3.229	0.5	ug/L	73286	1	6.242	713204	5.0
unknown-03	4.435	2.3	ug/L	330558	1	6.242	713204	5.0
2-Pentanone	6.769	0.6	ug/L	80921	1	6.242	713204	5.0
Pentanal	6.875	0.5	ug/L	75282	1	6.242	713204	5.0
Hexanal	8.782	0.5	ug/L	92192	2	9.412	874380	5.0
2-Heptanone	10.232	0.9	ug/L	159133	2	9.412	874380	5.0