LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU091724\
Data File : VU060856.D
Acq On : 18 Sep 2024 01:24
Operator : MD/SY
Sample : P3987-08
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH8P8

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\SFAMUTR091624WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU060856.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.599	87	96	105	rBV2	104727	128782	4.02%	1.033%
2	1.727	110	136	139	rBV4	46965	161362	5.03%	1.295%
3	1.785	148	154	172	rBV	108794	157359	4.91%	1.262%
4	1.911	188	193	211	rVB2	61051	100440	3.13%	0.806%
5	2.573	387	399	409	rBV4	327513	597052	18.63%	4.790%
6	2.647	409	422	470	rVV	908085	3205069	100.00%	25.713%
7	3.859	783	799	824	rBV	209677	507537	15.84%	4.072%
8	4.251	909	921	943	rBV5	13902	39057	1.22%	0.313%
9	4.653	1023	1046	1056	rBV3	137070	395145	12.33%	3.170%
10	4.708	1058	1063	1087	rVB	83837	224391	7.00%	1.800%
11	5.055	1154	1171	1194	rBV4	96683	271613	8.47%	2.179%
12	5.717	1359	1377	1394	rBV2	165497	431856	13.47%	3.465%
13	6.242	1527	1540	1570	rBV	161543	321050	10.02%	2.576%
14	6.537	1616	1632	1669	rBV3	665714	2861963	89.29%	22.961%
15	7.177	1813	1831	1859	rBV2	109996	220792	6.89%	1.771%
16	7.560	1939	1950	1968	rBV2	46345	85381	2.66%	0.685%
17	7.891	2042	2053	2069	rBV	201083	358227	11.18%	2.874%
18	8.174	2131	2141	2156	rBV3	27202	50423	1.57%	0.405%
19	8.566	2249	2263	2273	rBV	129083	226425	7.06%	1.817%
20	8.627	2273	2282	2322	rVB	199524	430823	13.44%	3.456%
21	8.830	2336	2345	2362	rVB	31789	54438	1.70%	0.437%
22	9.412	2514	2526	2547	rBV	244708	419496	13.09%	3.365%
23	10.749	2930	2942	2954	rBV2	77696	124791	3.89%	1.001%
24	11.367	3117	3134	3157	rBV	233560	379703	11.85%	3.046%
25	11.804	3259	3270	3291	rVV	237311	401815	12.54%	3.224%
26	12.187	3376	3389	3410	rBV	180235	309608	9.66%	2.484%

Sum of corrected areas: 12464598

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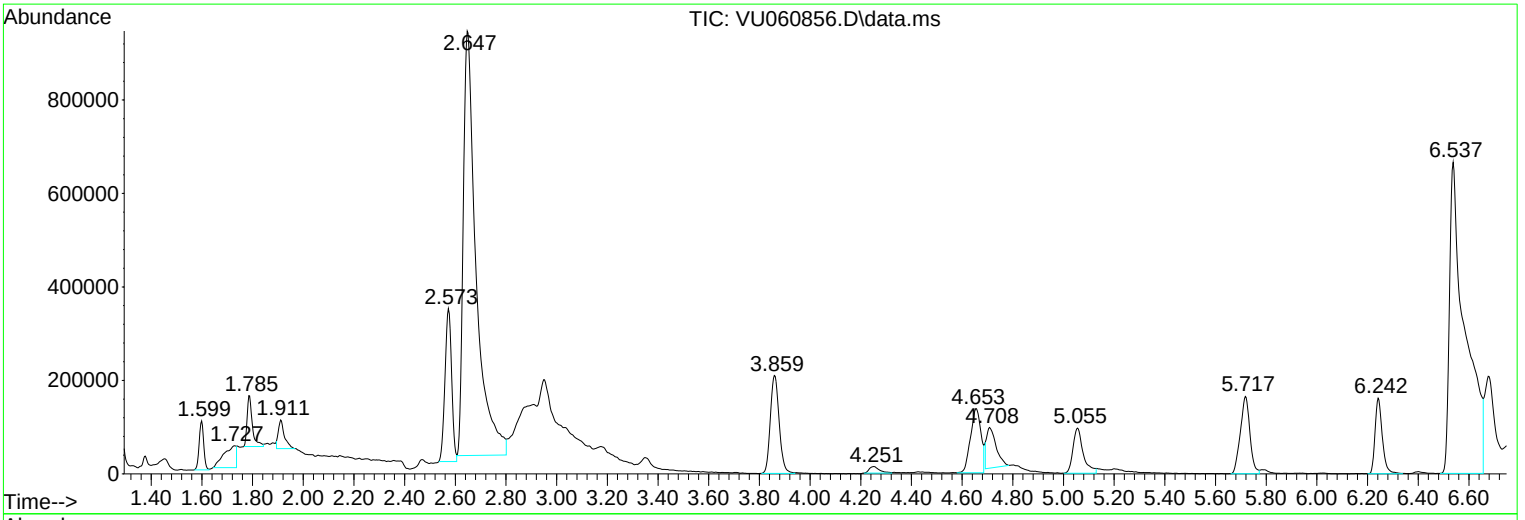
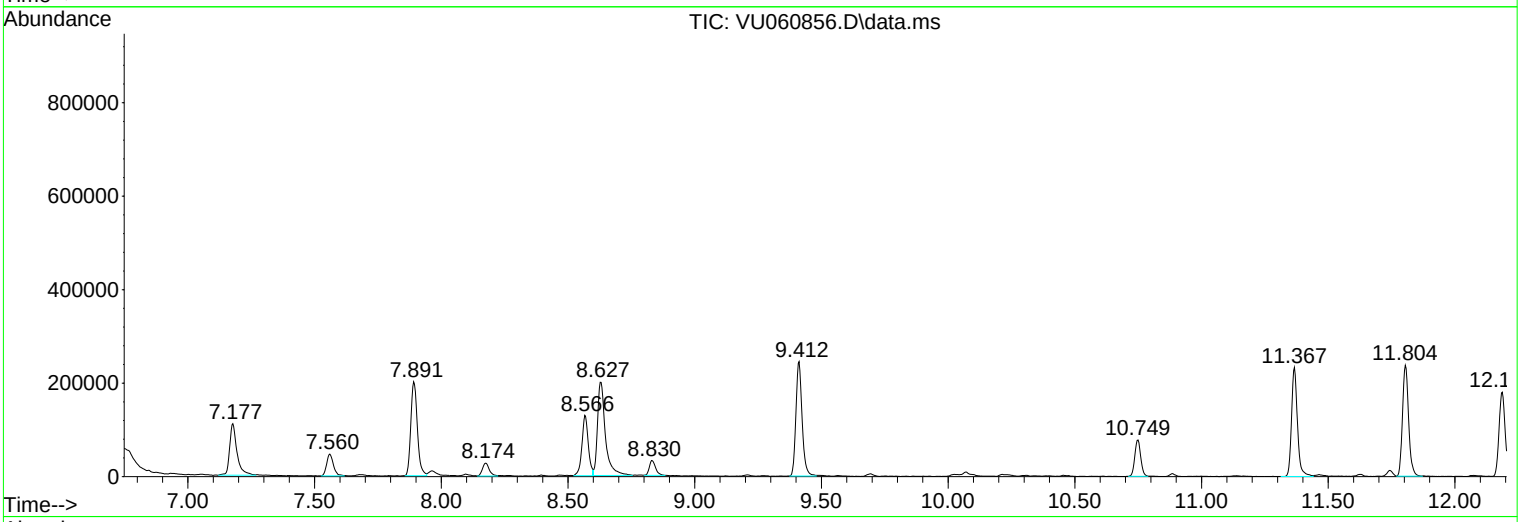
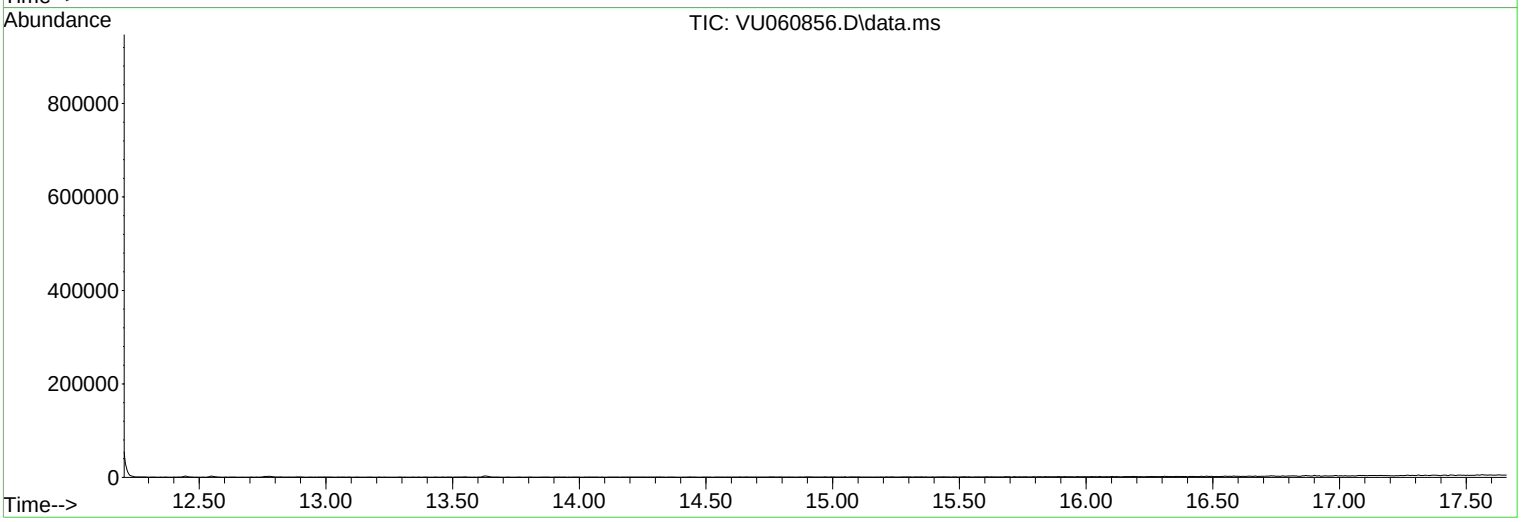
ClientSampleId :
BH8P8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091624WMA.M
Quant Title : TRACE VOA SFAM1.0

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







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Quant Title : TRACE VOA SFAM1.0

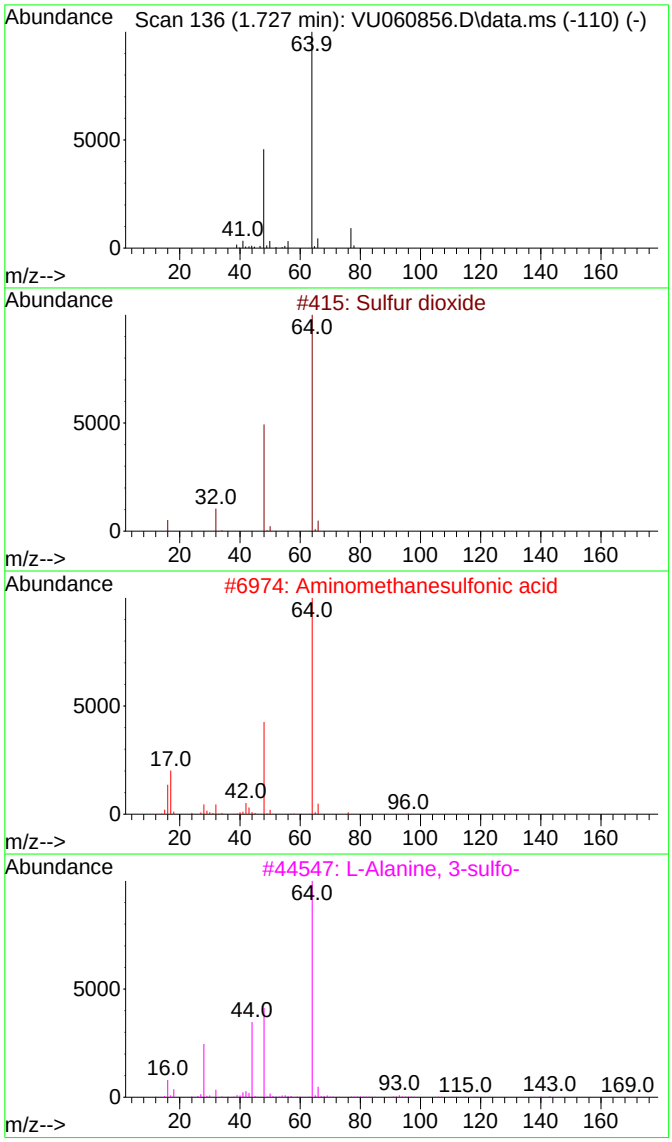
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

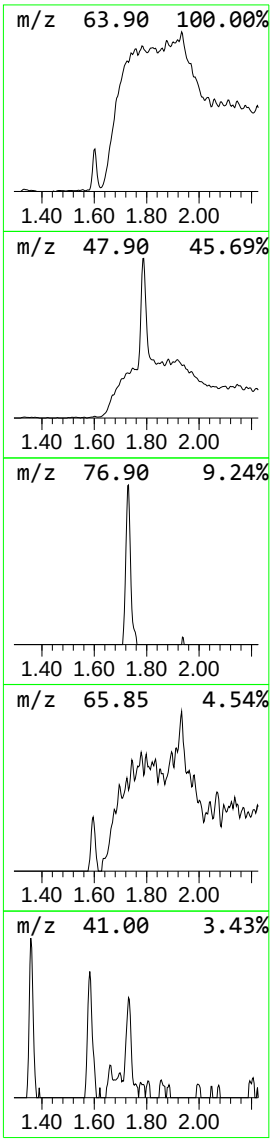
****

Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.727	2.51 ug/L	161362	1,4-Difluorobenzene	6.242

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	Sulfur dioxide	64	O2S	007446-09-5	5





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Data File : VU060856.D
Acq On : 18 Sep 2024 01:24
Operator : MD/SY
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ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH8P8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091624WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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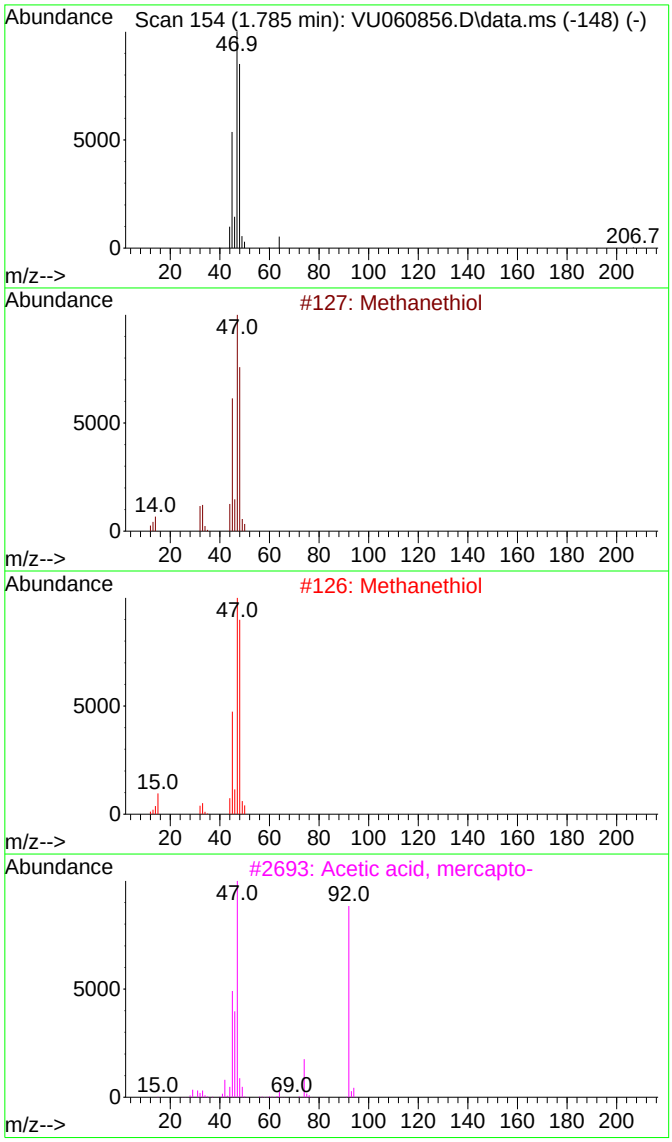
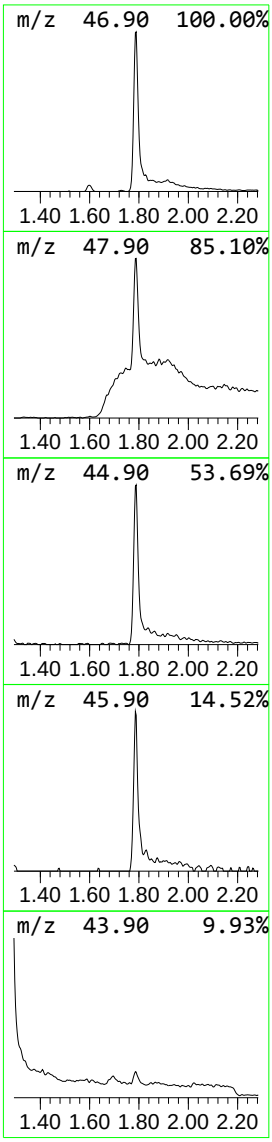
Peak Number 2 Methanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.785	2.45 ug/L	157359	1,4-Difluorobenzene	6.242

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethiol	48	CH4S	000074-93-1	91
2	Methanethiol	48	CH4S	000074-93-1	90
3	Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	28
4	3-Mercaptopropionitrile	87	C3H5NS	001001-58-7	25
5	Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	9





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Operator : MD/SY
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ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH8P8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091624WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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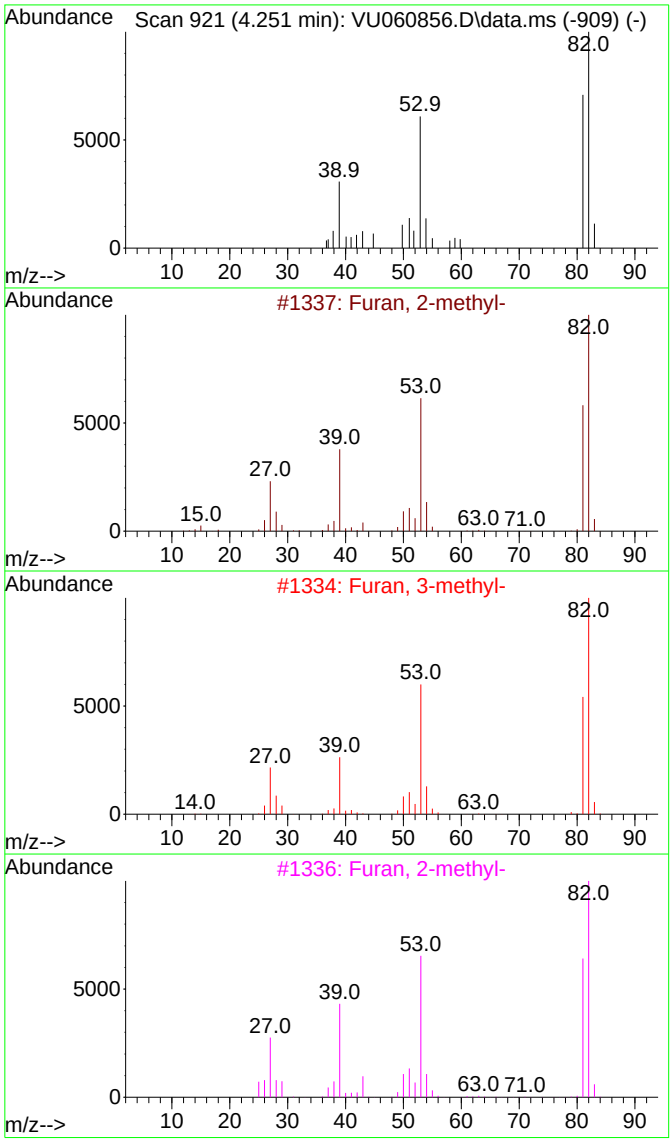
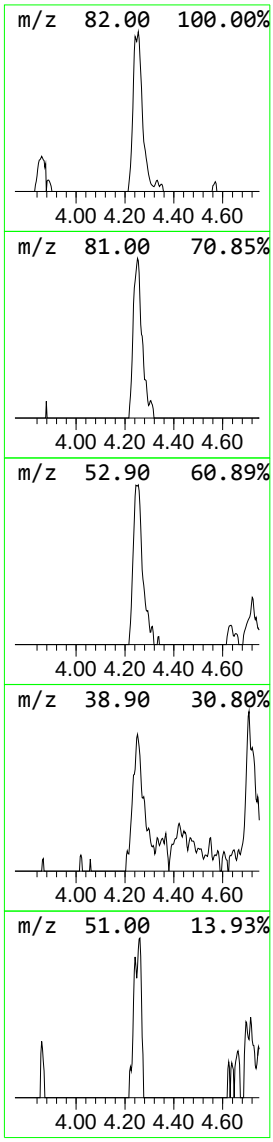
Peak Number 3 Furan, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.251	0.61 ug/L	39057	1,4-Difluorobenzene	6.242

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, 2-methyl-	82	C5H6O	000534-22-5	91
2	Furan, 3-methyl-	82	C5H6O	000930-27-8	91
3	Furan, 2-methyl-	82	C5H6O	000534-22-5	91
4	Furan, 2-methyl-	82	C5H6O	000534-22-5	86
5	Furan, 2-methyl-	82	C5H6O	000534-22-5	72





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ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH8P8

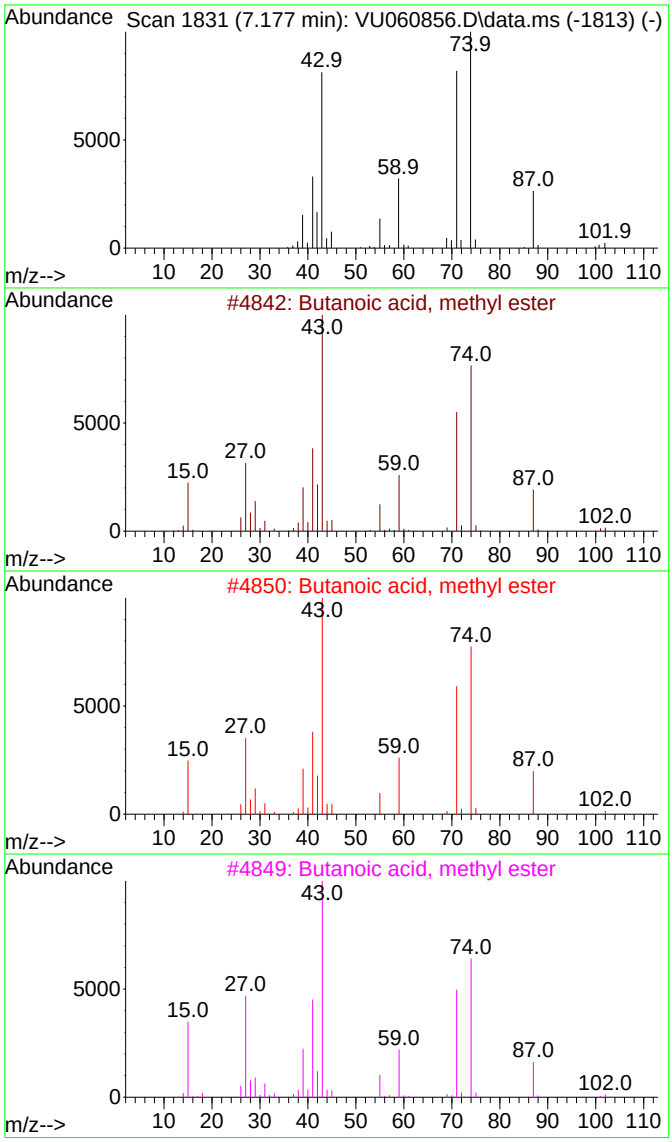
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091624WMA.M
Quant Title : TRACE VOA SFAM1.0

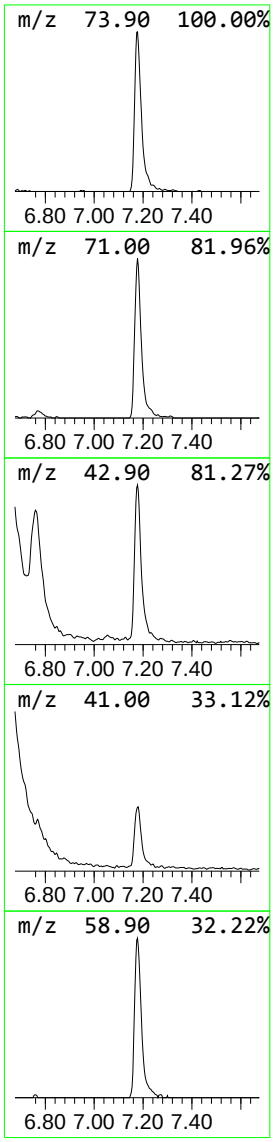
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butanoic acid, methyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.177	3.44 ug/L	220792	1,4-Difluorobenzene	6.242

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	91
2	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	91
3	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	91
4	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	47
5	2,3,4-Trimethylpentanoic acid	144	C8H16O2	090435-18-0	45





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ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_U
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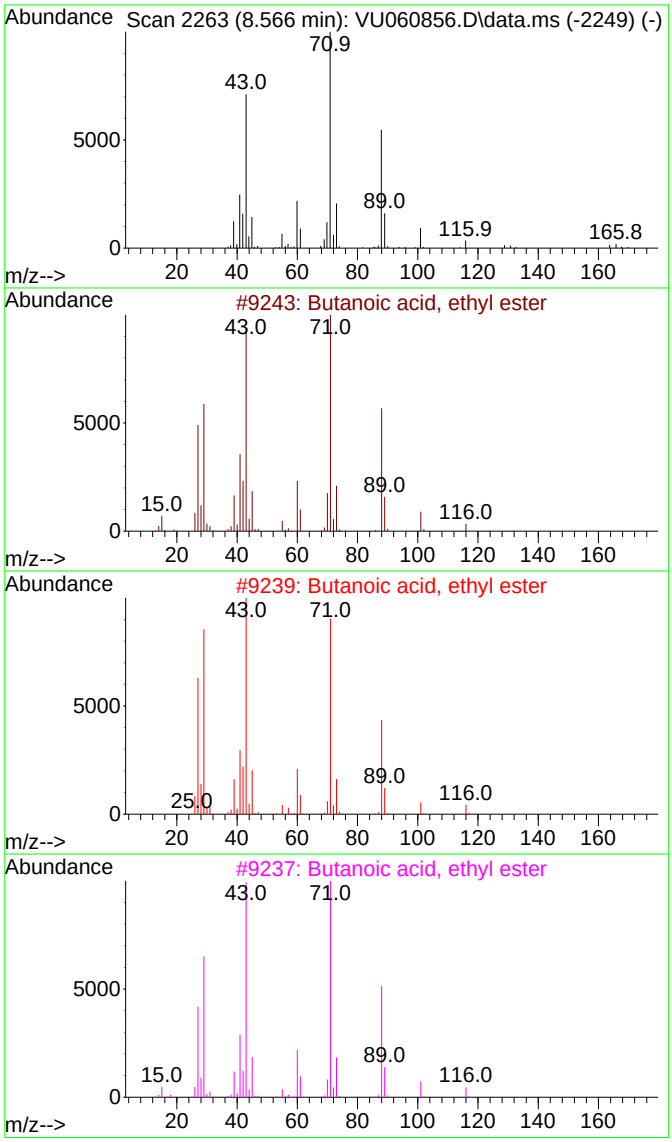
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091624WMA.M
Quant Title : TRACE VOA SFAM1.0

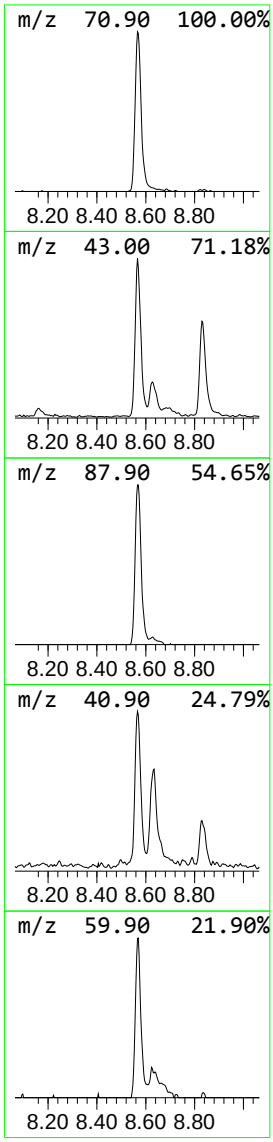
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Butanoic acid, ethyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.566	2.70 ug/L	226425	Chlorobenzene-d5	9.412

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	96
2	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	94
3	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	94
4	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	86
5	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	83





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091624WMA.M
Quant Title : TRACE VOA SFAM1.0

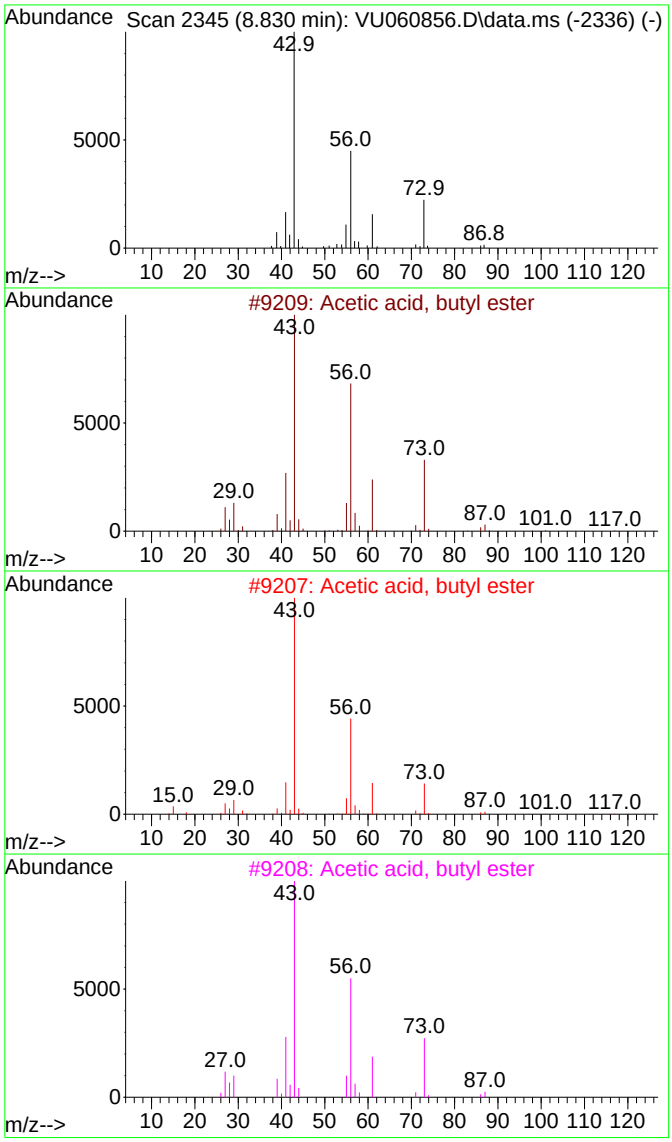
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

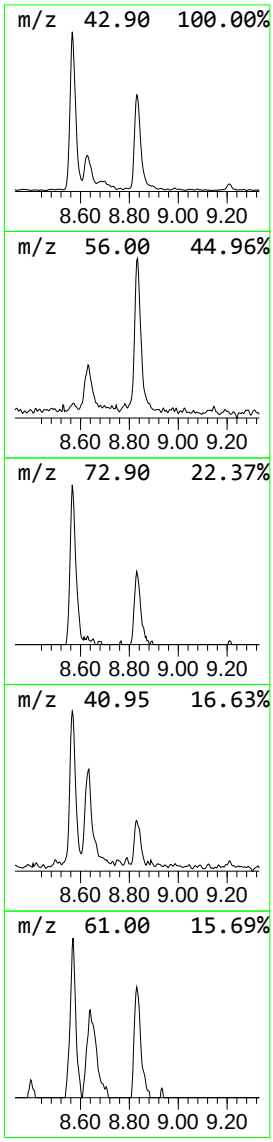
****

Peak Number 7 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.830	0.65 ug/L	54438	Chlorobenzene-d5	9.412

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
2	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
3	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
4	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	40
5	Isobutyl acetate	116	C6H12O2	000110-19-0	39





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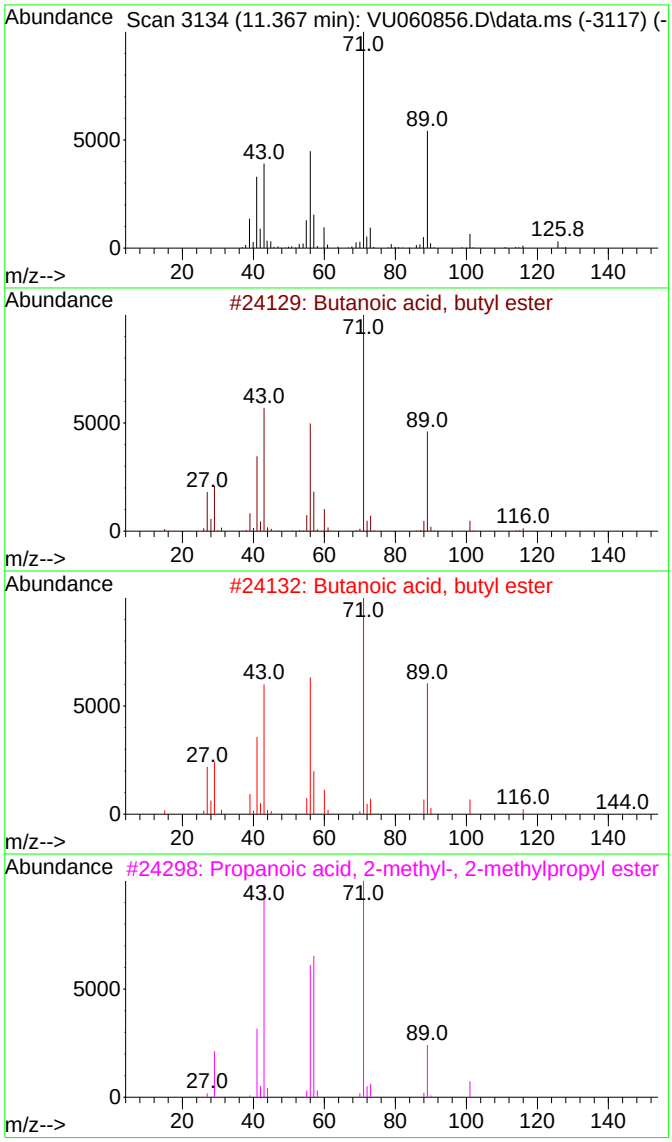
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091624WMA.M
Quant Title : TRACE VOA SFAM1.0

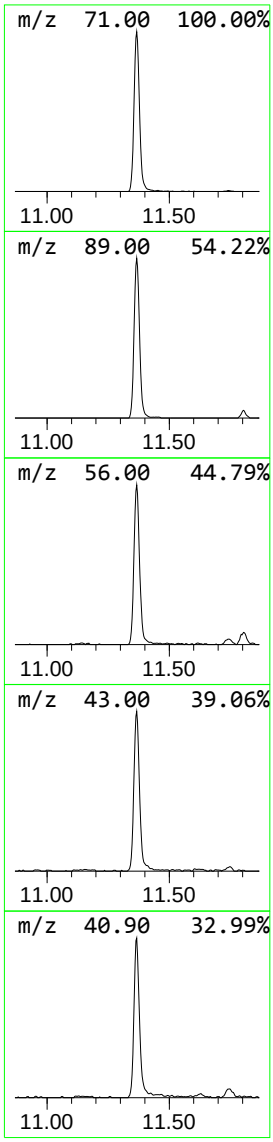
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.367	4.72 ug/L	379703	1,4-Dichlorobenzene-d4	11.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90
2	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	83
3	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	72
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	72
5	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.727	2.5	ug/L	161362	1	6.242	321050	5.0
Methanethiol	1.785	2.5	ug/L	157359	1	6.242	321050	5.0
Furan, 2-methyl-	4.251	0.6	ug/L	39057	1	6.242	321050	5.0
Butanoic acid, ...	7.177	3.4	ug/L	220792	1	6.242	321050	5.0
Butanoic acid, ...	8.566	2.7	ug/L	226425	2	9.412	419496	5.0
Acetic acid, bu...	8.830	0.7	ug/L	54438	2	9.412	419496	5.0
Butanoic acid, ...	11.367	4.7	ug/L	379703	3	11.804	401815	5.0