

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011323\
 Data File : VU052680.D
 Acq On : 13 Jan 2023 15:27
 Operator : JC/MD
 Sample : 01139-04
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH1Y7

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\SFAMUTR011023WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU052666.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.472	339	352	367	rBV	2396943	4114730	10.00%	4.025%
2	3.224	579	586	611	rVB2	188044	423053	1.03%	0.414%
3	4.662	1017	1033	1038	rBV2	399066	849514	2.06%	0.831%
4	4.723	1039	1052	1133	rVB	1978270	9187030	22.32%	8.986%
5	5.060	1143	1157	1170	rBV2	178867	573212	1.39%	0.561%
6	5.723	1340	1363	1375	rBV2	232951	609147	1.48%	0.596%
7	6.633	1599	1646	1679	rBV3	4749741	41152922	100.00%	40.251%
8	6.858	1707	1716	1737	rVB	1087050	2074100	5.04%	2.029%
9	7.179	1806	1816	1840	rVB	438404	819925	1.99%	0.802%
10	7.893	2027	2038	2053	rVB	294573	509599	1.24%	0.498%
11	8.153	2106	2119	2164	rVB	2474662	4291369	10.43%	4.197%
12	8.571	2237	2249	2260	rBV	1722276	2719071	6.61%	2.660%
13	8.632	2260	2268	2292	rVB	346116	666078	1.62%	0.651%
14	8.829	2318	2329	2367	rVB	1046247	1719448	4.18%	1.682%
15	9.276	2451	2468	2500	rBV2	558135	1595476	3.88%	1.561%
16	9.414	2500	2511	2545	rVB	281525	511939	1.24%	0.501%
17	10.575	2858	2872	2898	rBV	895037	1773603	4.31%	1.735%
18	10.960	2980	2992	3014	rBV	1261810	1851989	4.50%	1.811%
19	11.153	3040	3052	3075	rBV	866080	1292966	3.14%	1.265%
20	11.372	3104	3120	3144	rBV	13899080	19871634	48.29%	19.436%
21	11.809	3244	3256	3272	rBV	343423	543921	1.32%	0.532%
22	12.189	3357	3374	3388	rBV2	283942	522201	1.27%	0.511%
23	12.999	3614	3626	3649	rBV	454321	716564	1.74%	0.701%
24	13.298	3707	3719	3739	rBV	1491179	2163735	5.26%	2.116%
25	13.401	3739	3751	3779	rVB	524907	900551	2.19%	0.881%
26	15.397	4360	4372	4393	rBV	504624	785786	1.91%	0.769%

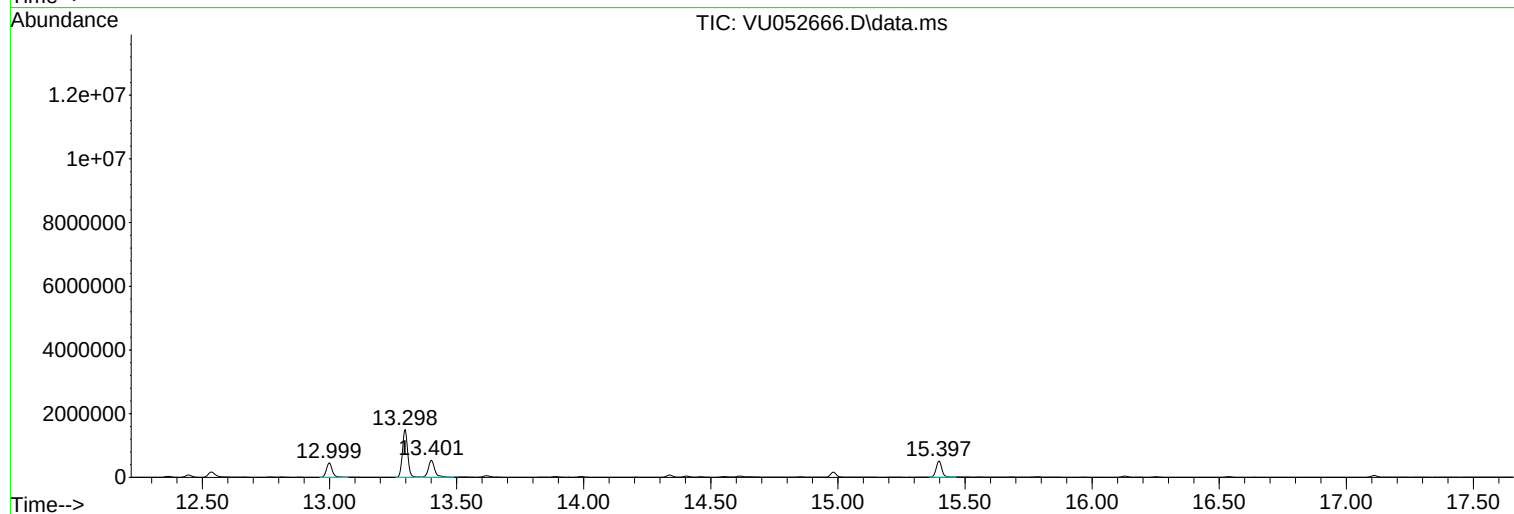
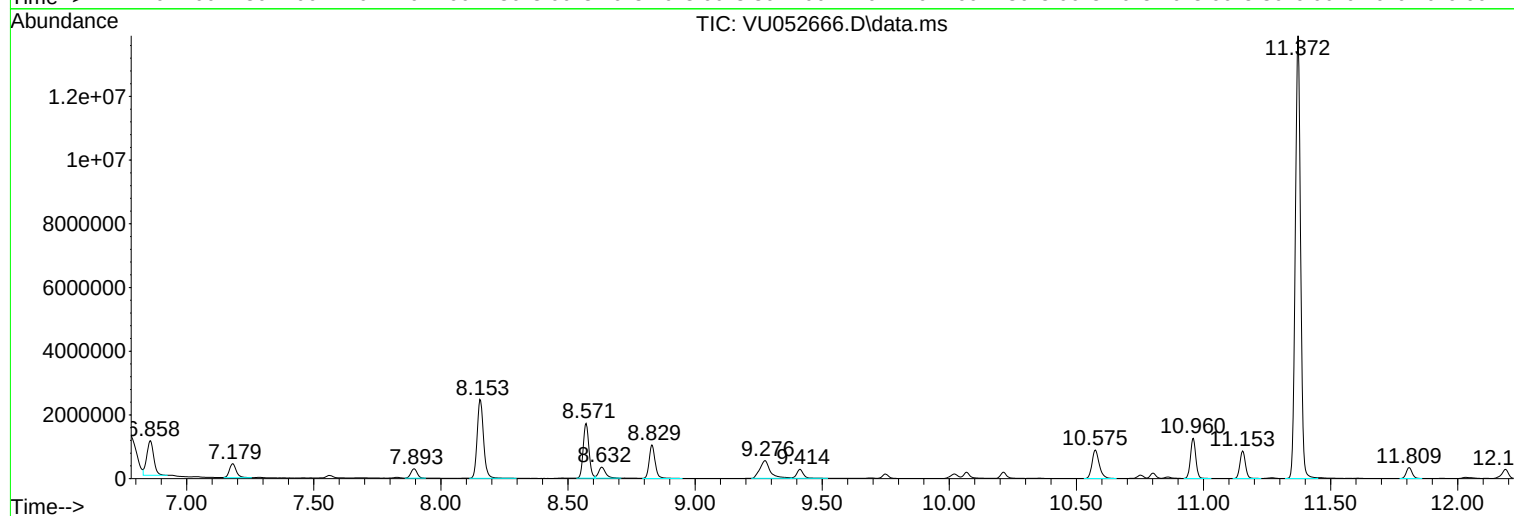
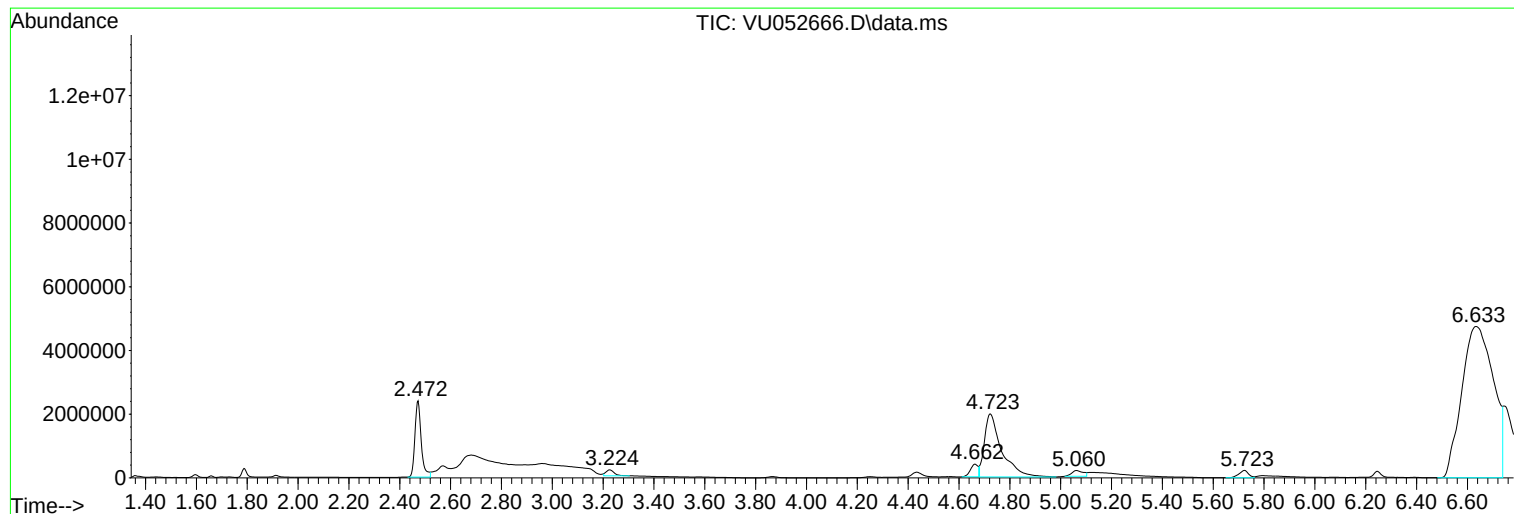
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ClientSampleId :
BH1Y7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011023WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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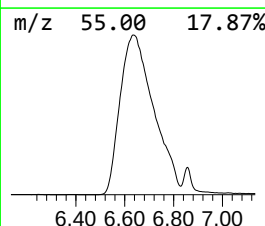
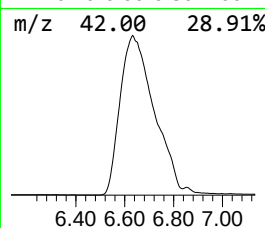
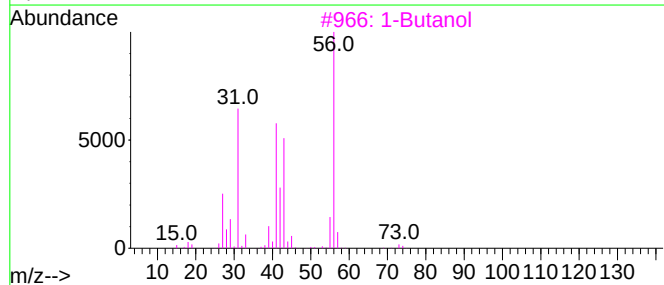
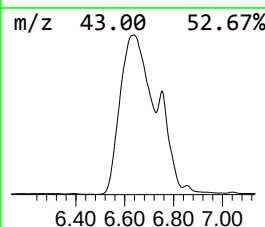
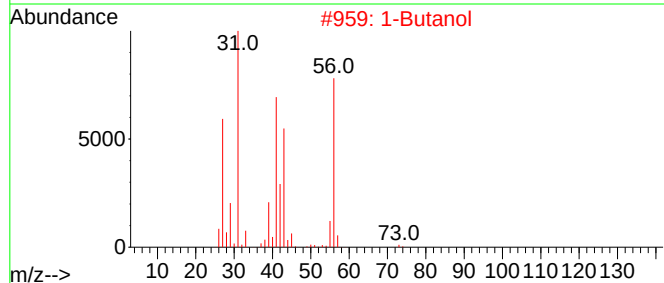
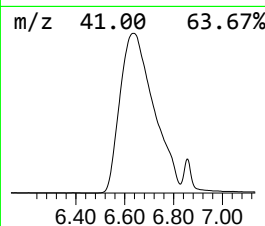
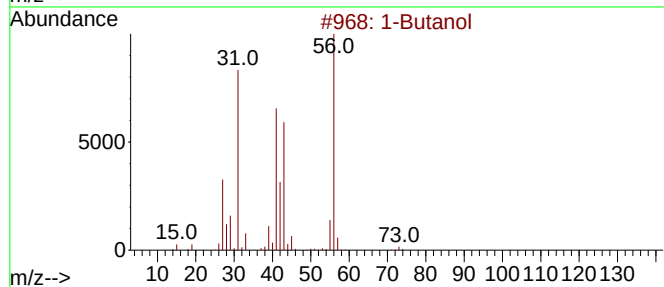
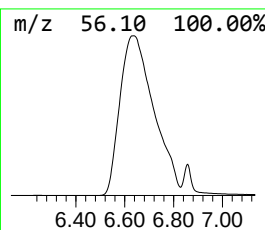
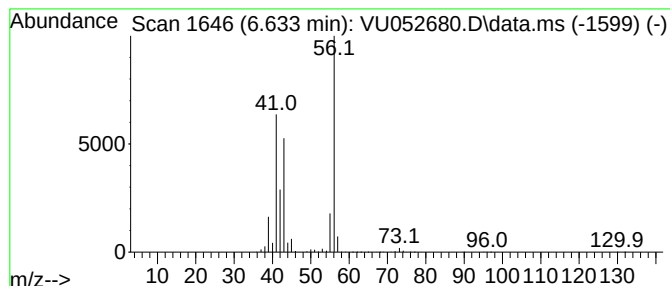
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 1-Butanol Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.633	5.00 ug/L	41152900	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol			74	C4H10O	000071-36-3	91
2	1-Butanol			74	C4H10O	000071-36-3	86
3	1-Butanol			74	C4H10O	000071-36-3	83
4	1-Butanol			74	C4H10O	000071-36-3	58
5	1-Butanol			74	C4H10O	000071-36-3	52



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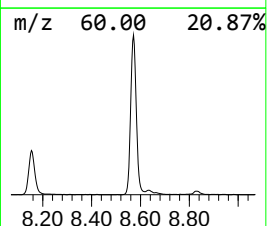
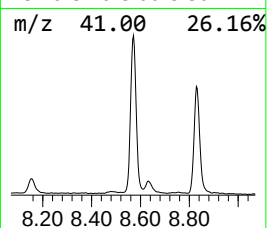
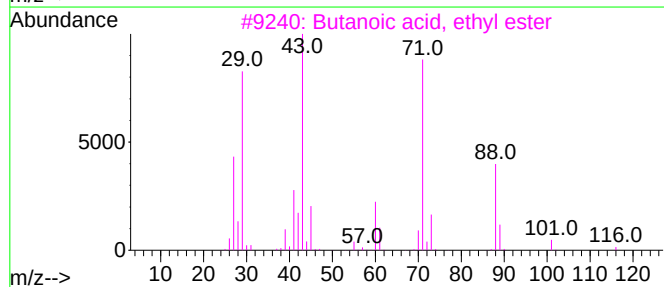
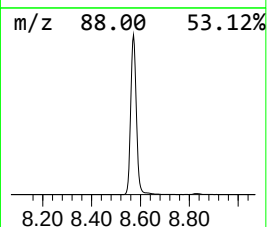
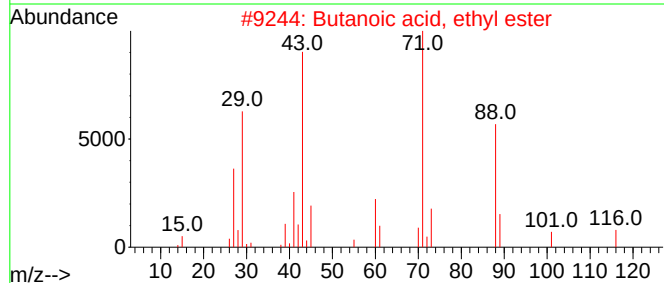
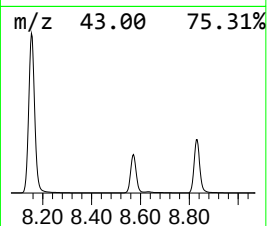
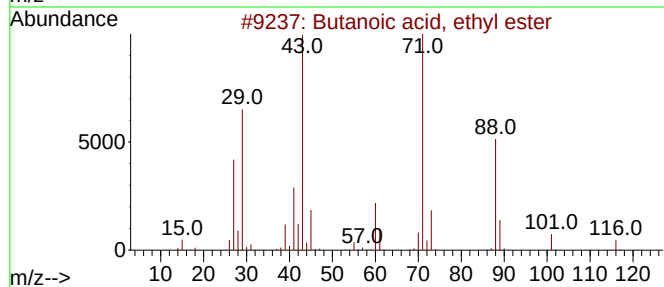
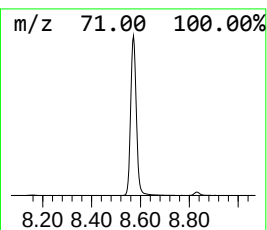
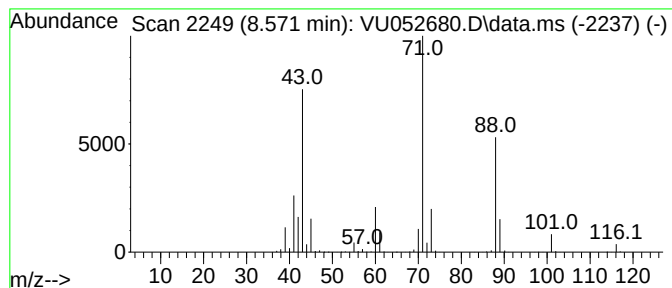
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011023WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
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Peak Number 2 Butanoic acid, ethyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.571	26.56 ug/L	2719070	Chlorobenzene-d5	9.414

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	97
2			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	90
3			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	83
4			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	81
5			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	64



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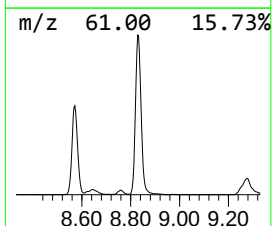
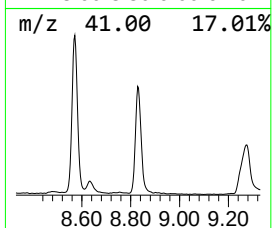
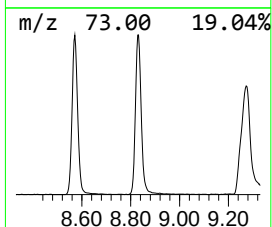
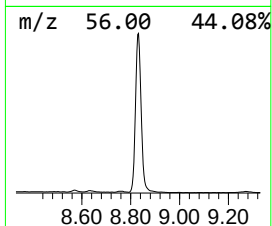
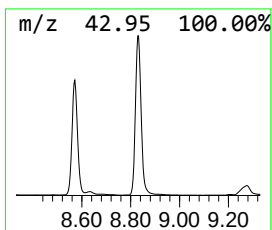
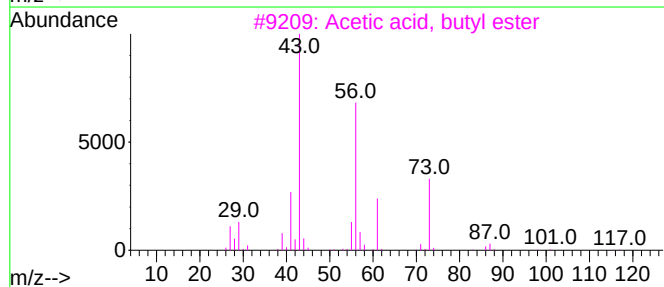
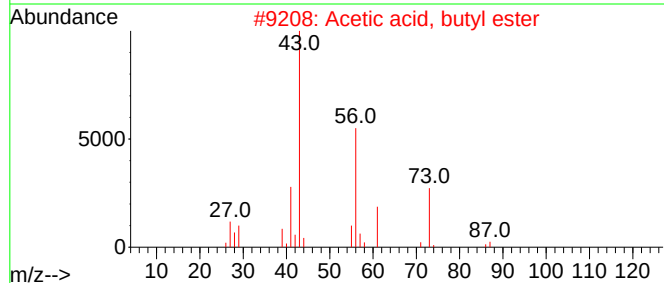
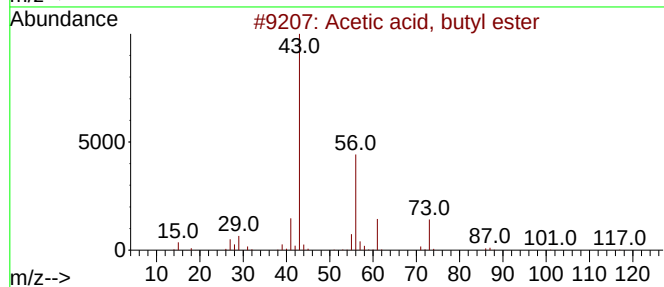
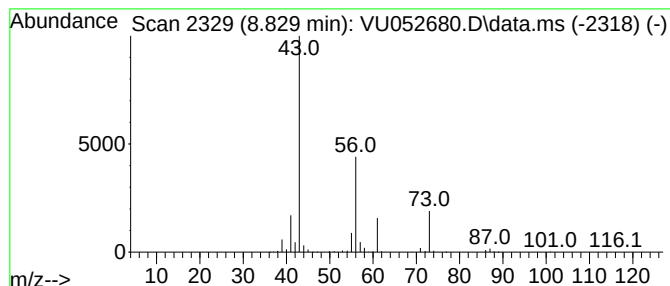
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.829	16.79 ug/L	1719450	Chlorobenzene-d5	9.414

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
5			Isobutyl acetate	116	C6H12O2	000110-19-0	40



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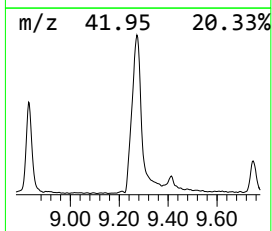
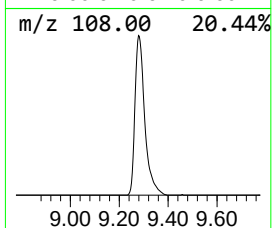
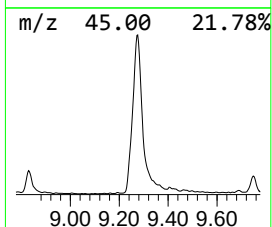
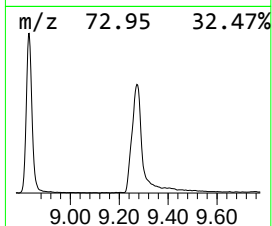
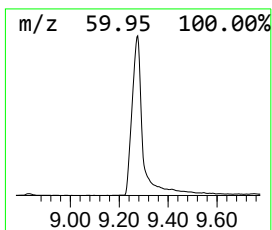
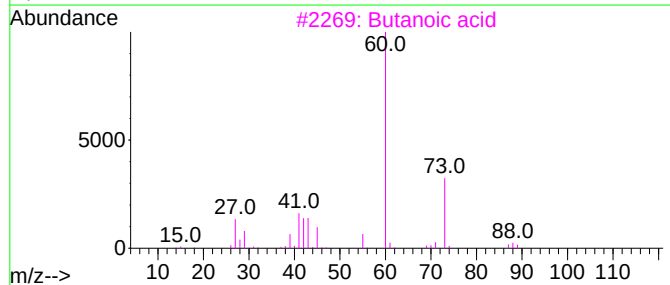
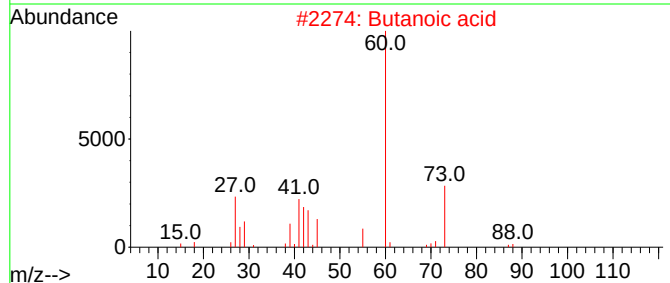
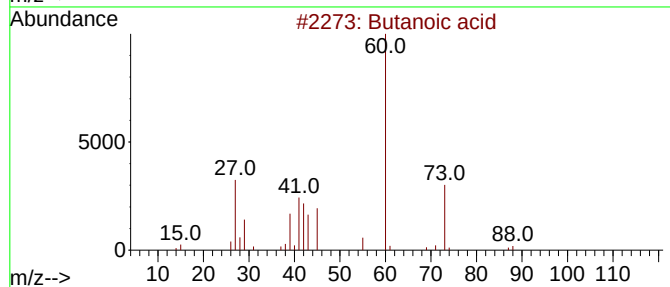
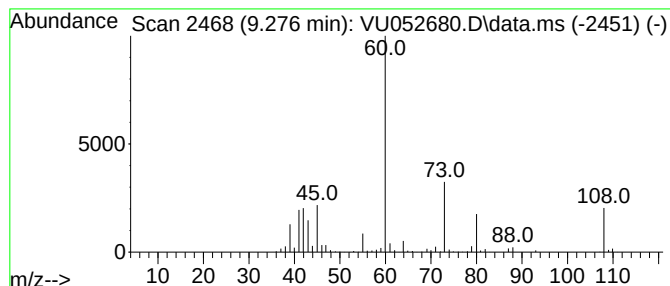
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Butanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.276	15.58 ug/L	1595480	Chlorobenzene-d5	9.414

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid	88	C4H8O2	000107-92-6	76
2			Butanoic acid	88	C4H8O2	000107-92-6	62
3			Butanoic acid	88	C4H8O2	000107-92-6	52
4			Butanoic acid	88	C4H8O2	000107-92-6	52
5			Hexanoic acid	116	C6H12O2	000142-62-1	42



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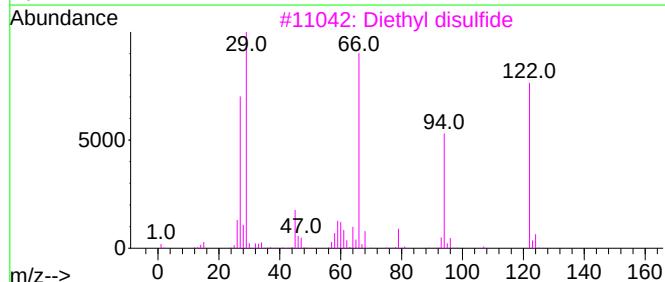
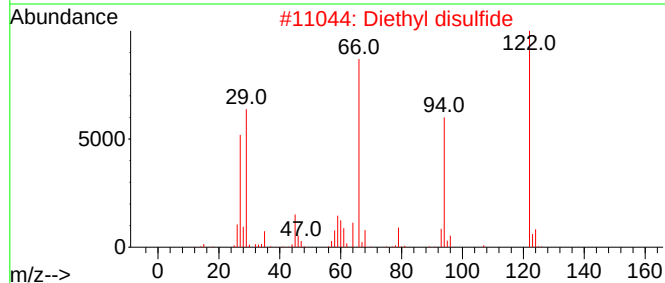
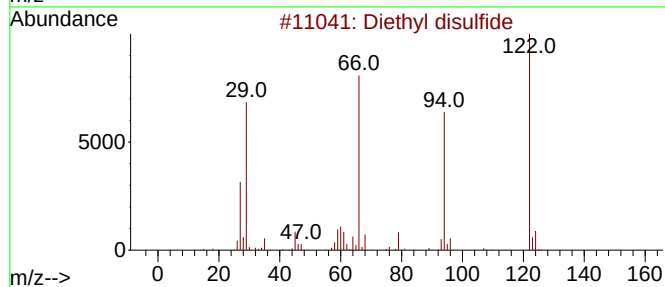
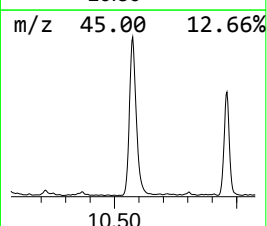
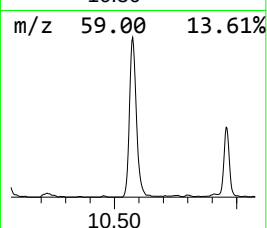
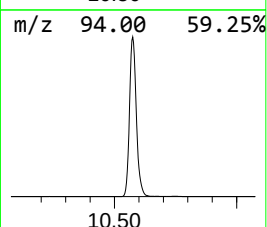
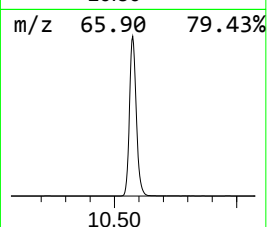
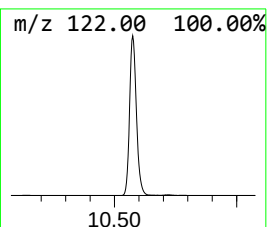
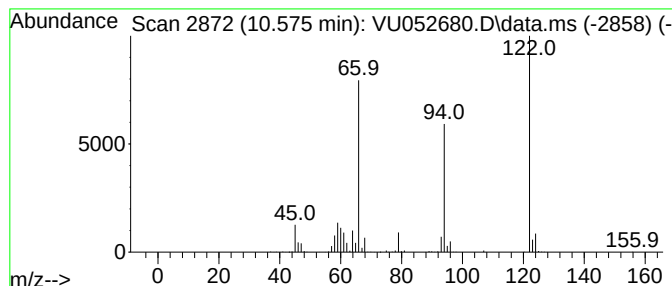
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Diethyl disulfide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.575	17.32 ug/L	1773600	Chlorobenzene-d5	9.414

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethyl disulfide	122	C4H10S2	000110-81-6	97
2			Diethyl disulfide	122	C4H10S2	000110-81-6	95
3			Diethyl disulfide	122	C4H10S2	000110-81-6	91
4			Benzene, ethoxy-	122	C8H10O	000103-73-1	50
5			Diethyl sulfone	122	C4H10O2S	000597-35-3	42



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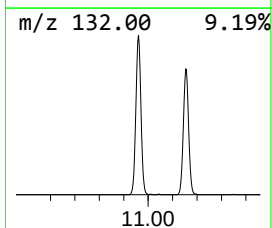
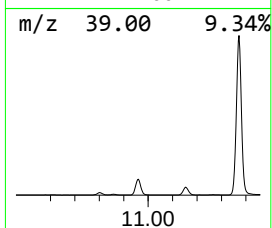
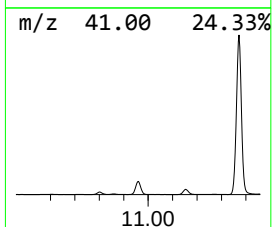
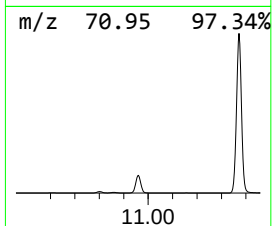
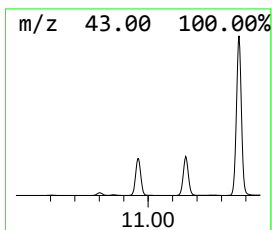
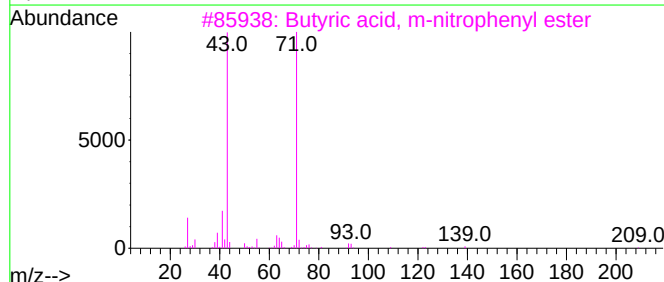
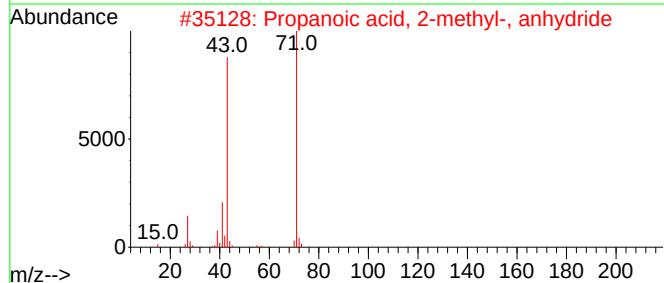
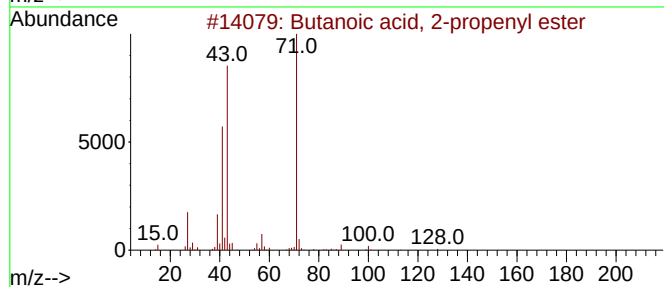
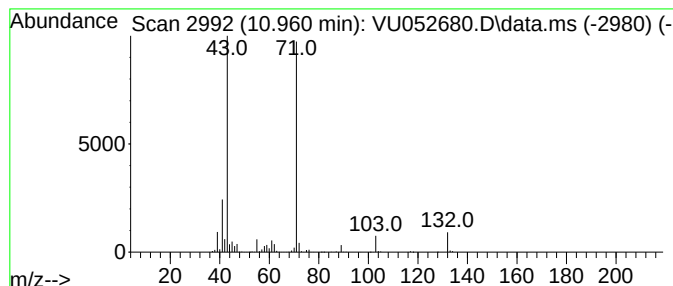
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Butanoic acid, 2-propenyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.960	17.02 ug/L	1851990	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 2-propenyl ester	128	C7H12O2	002051-78-7	59
2			Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	59
3			Butyric acid, m-nitrophenyl ester	209	C10H11NO4	014617-97-1	59
4			2-Hydroperoxytetrahydrofuran, TM...	176	C7H16O3Si	1000368-50-8	50
5			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011323\
Data File : VU052680.D
Acq On : 13 Jan 2023 15:27
Operator : JC/MD
Sample : 01139-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH1Y7

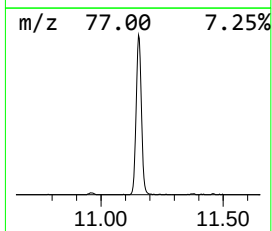
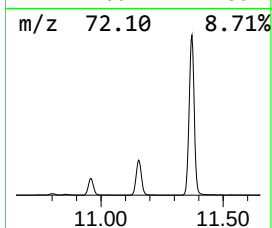
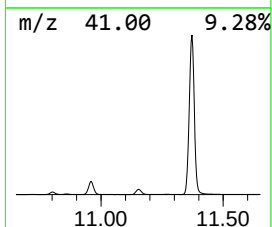
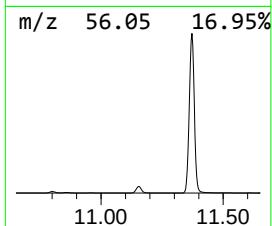
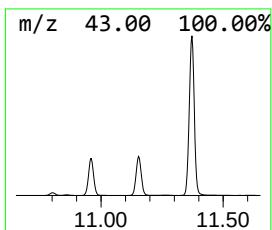
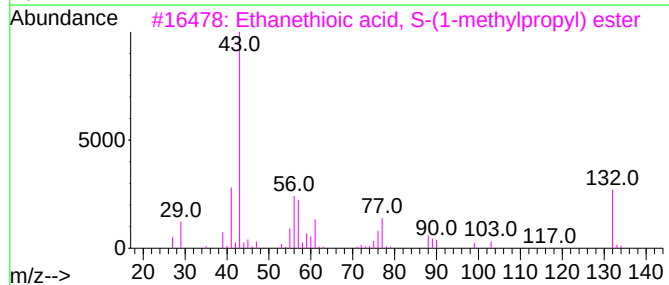
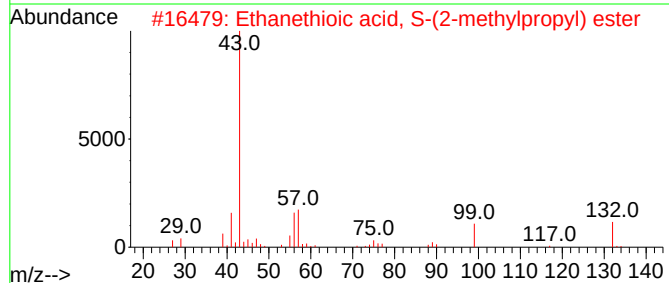
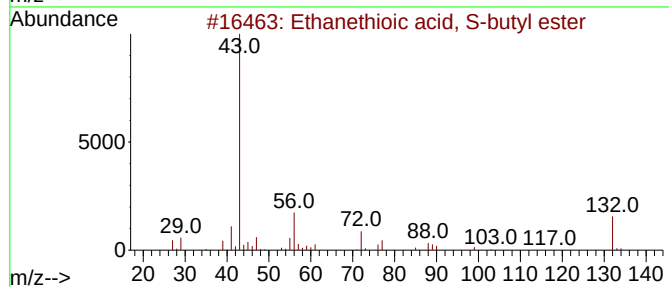
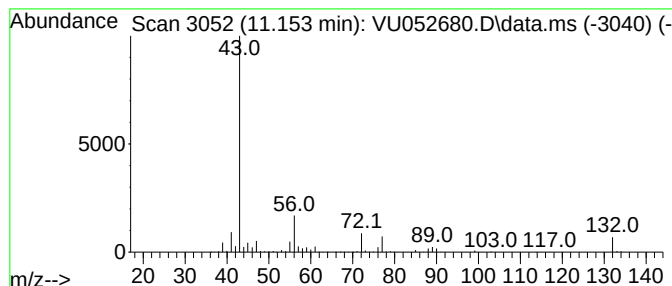
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 Ethanethioic acid, S-butyl ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.153	11.89 ug/L	1292970	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanethioic acid, S-butyl ester	132	C6H12OS	000928-47-2	91
2			Ethanethioic acid, S-(2-methylpr...	132	C6H12OS	002432-37-3	59
3			Ethanethioic acid, S-(1-methylpr...	132	C6H12OS	002432-39-5	42
4			2,3-Epoxybutane	72	C4H8O	003266-23-7	25
5			Acetyl 2-formylethyl sulfide	132	C5H8O2S	053943-93-4	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011323\
Data File : VU052680.D
Acq On : 13 Jan 2023 15:27
Operator : JC/MD
Sample : 01139-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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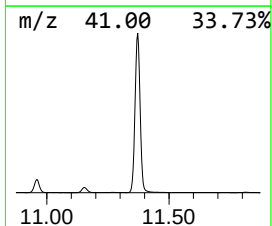
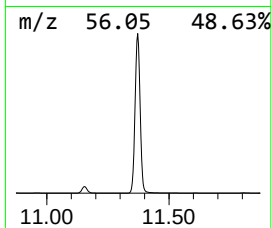
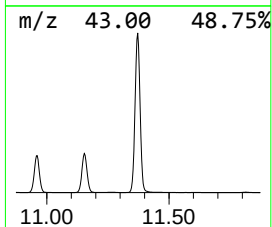
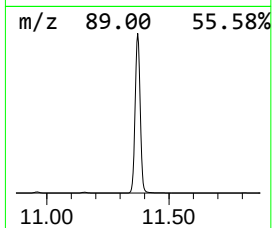
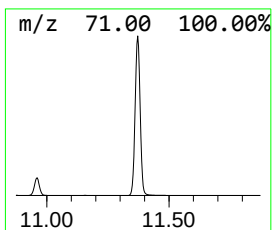
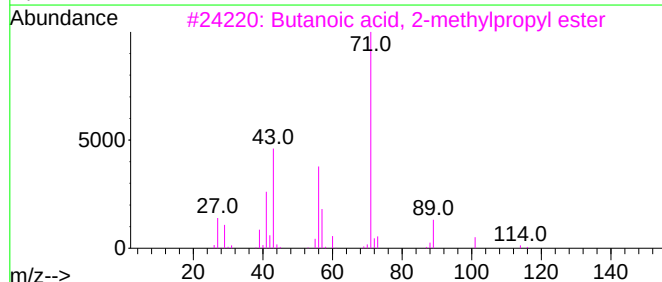
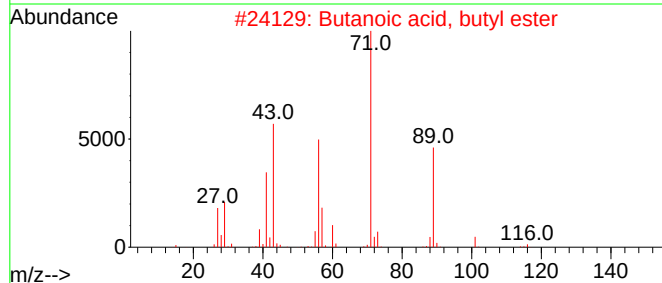
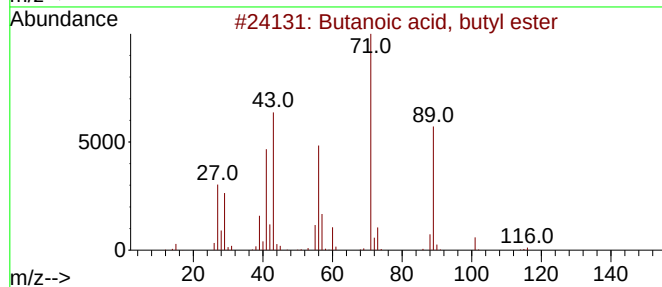
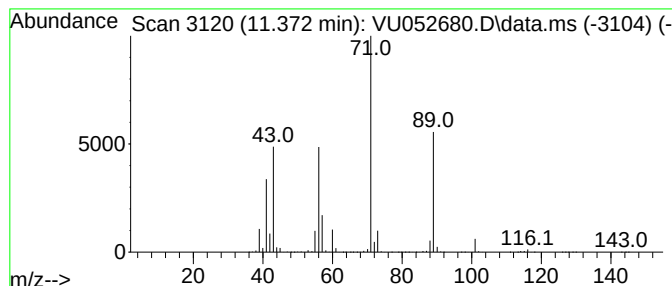
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Quant Title : TRACE VOA SFAM1.0

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.
11.372	182.67 ug/L	19871600	1,4-Dichlorobenzene-d4	11.809

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	90
3			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
4			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	72
5			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011323\
Data File : VU052680.D
Acq On : 13 Jan 2023 15:27
Operator : JC/MD
Sample : 01139-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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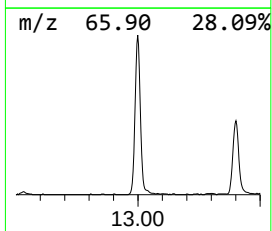
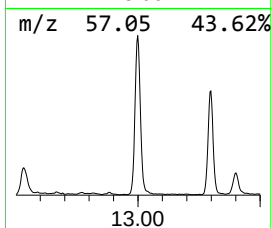
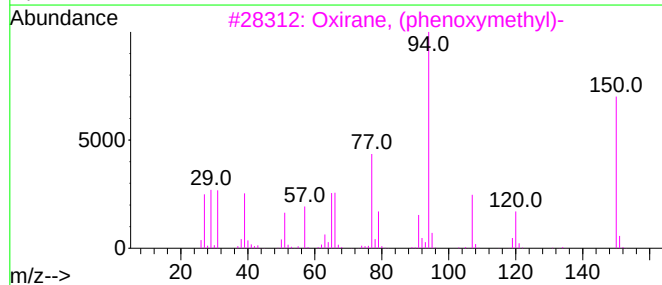
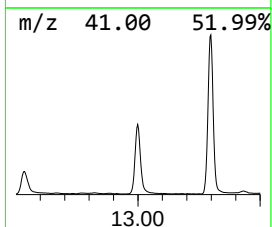
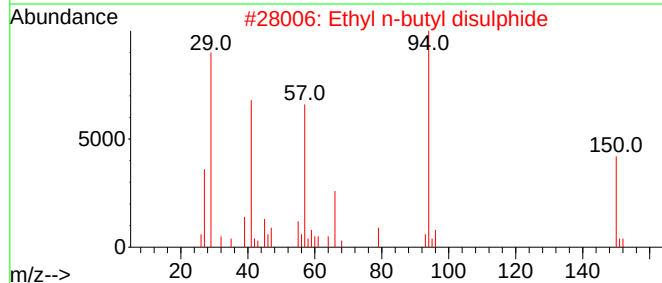
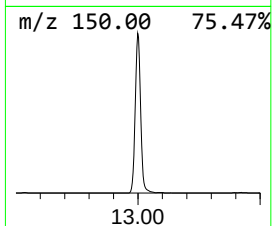
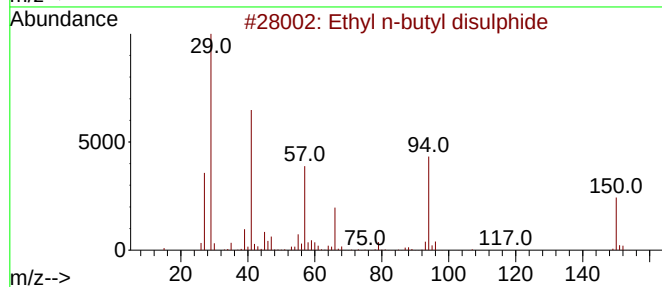
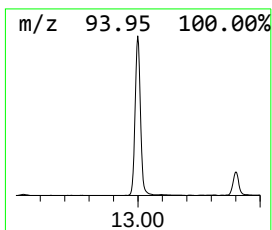
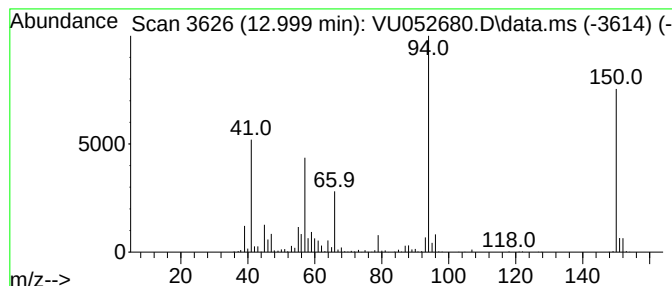
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 Ethyl n-butyl disulphide Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.999	6.59 ug/L	716564	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl n-butyl disulphide	150	C6H14S2	063986-03-8	91
2			Ethyl n-butyl disulphide	150	C6H14S2	063986-03-8	72
3			Oxirane, (phenoxymethyl)-	150	C9H10O2	000122-60-1	56
4			Disulfide, ethyl 1-methylpropyl	150	C6H14S2	054166-53-9	53
5			Phenol	94	C6H6O	000108-95-2	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011323\
Data File : VU052680.D
Acq On : 13 Jan 2023 15:27
Operator : JC/MD
Sample : 01139-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
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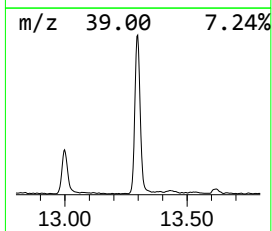
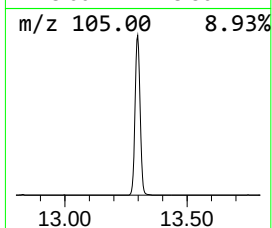
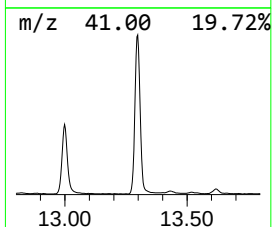
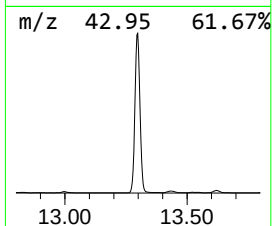
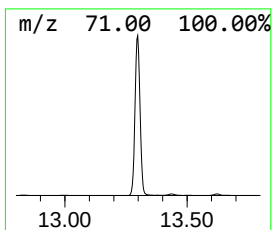
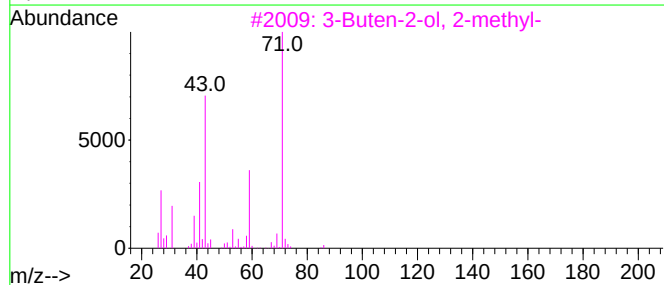
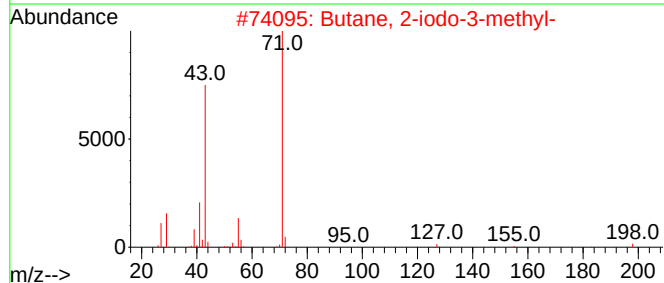
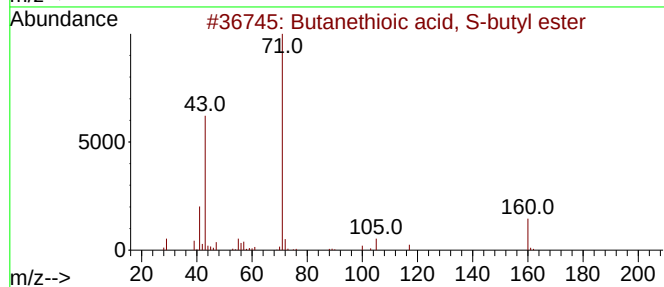
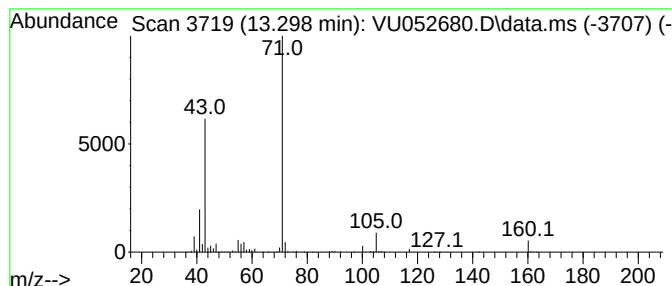
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 10 Butanethioic acid, S-butyl ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.298	19.89 ug/L	2163740	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanethioic acid, S-butyl ester	160	C8H16OS	002432-52-2	91
2			Butane, 2-iodo-3-methyl-	198	C5H11I	018295-27-7	59
3			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	45
4			Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	45
5			Butanethioic acid, S-(1,1-dimeth...	160	C8H16OS	006330-43-4	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011323\
Data File : VU052680.D
Acq On : 13 Jan 2023 15:27
Operator : JC/MD
Sample : 01139-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH1Y7

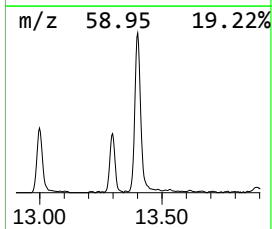
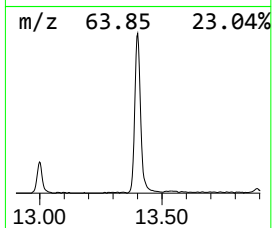
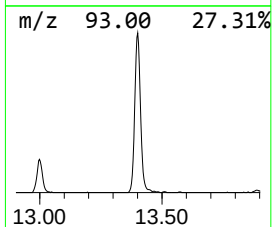
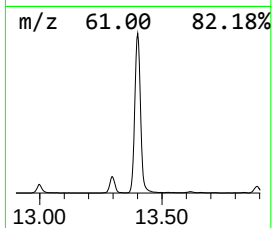
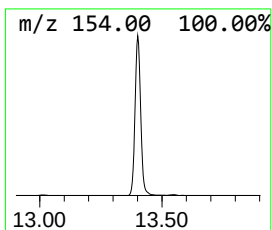
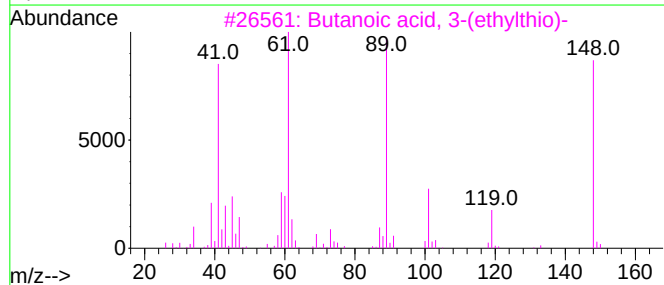
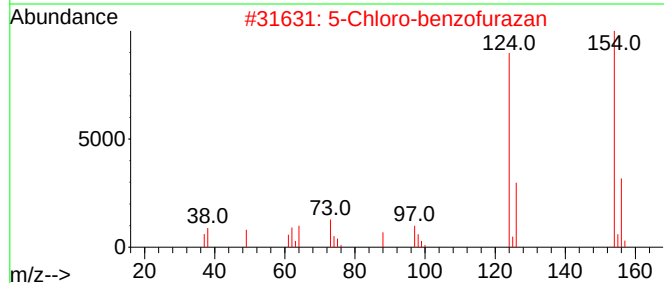
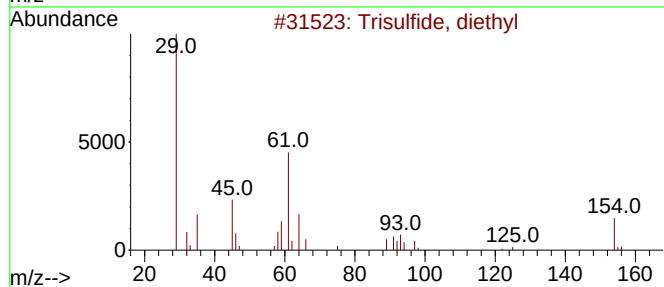
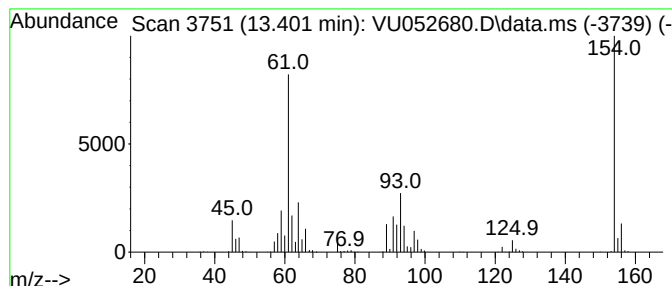
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 11 unknown-01 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.401	8.28 ug/L	900551	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trisulfide, diethyl	154	C4H10S3	003600-24-6	38
2			5-Chloro-benzofurazan	154	C6H3ClN2O	019155-86-3	35
3			Butanoic acid, 3-(ethylthio)-	148	C6H12O2S	089534-40-7	17
4			2-Hydrazinyl-5-nitropyridine	154	C5H6N4O2	006343-98-2	12
5			N-Trifluoroacetyl-phenentermine	245	C12H14F3NO	042524-63-0	12



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011323\
Data File : VU052680.D
Acq On : 13 Jan 2023 15:27
Operator : JC/MD
Sample : 01139-04
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ALS Vial : 13 Sample Multiplier: 1

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ClientSampleId :
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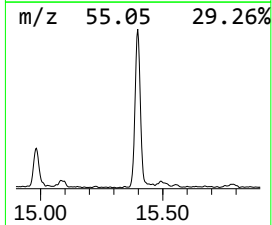
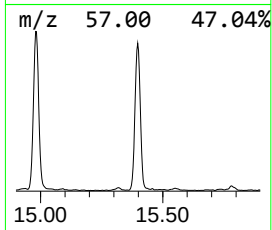
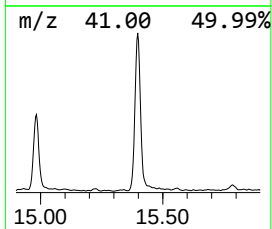
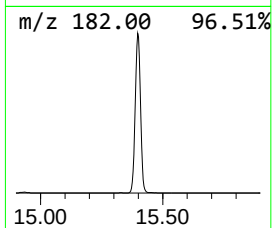
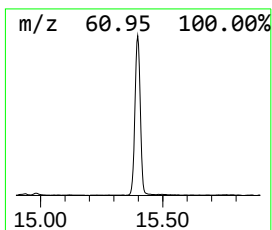
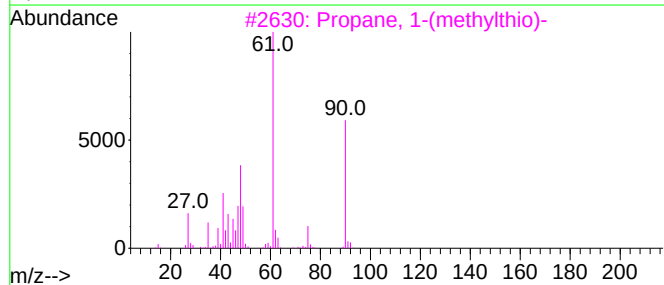
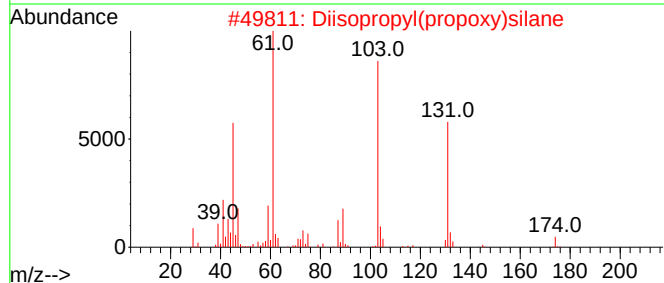
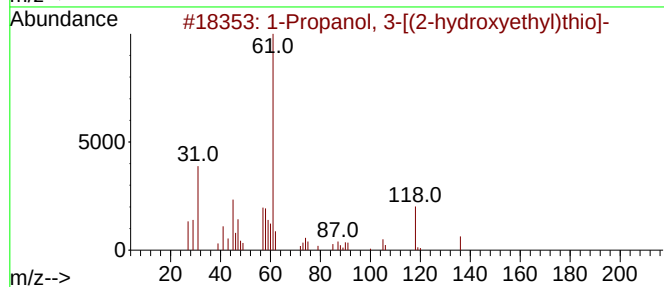
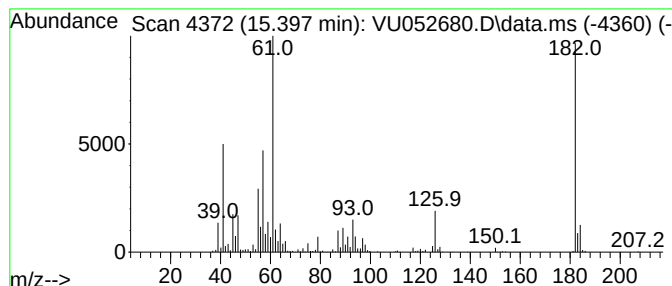
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 12 unknown-02 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.398	7.22 ug/L	785786	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol, 3-[(2-hydroxyethyl)thio]-	136	C5H12O2S	005323-60-4	32
2			Diisopropyl(propoxy)silane	174	C9H22OSi	167567-63-7	25
3			Propane, 1-(methylthio)-	90	C4H10S	003877-15-4	25
4			Disulfide, bis(2-sulfhydrylethyl)-	186	C4H10S4	010008-38-5	22
5			Trisulfide, dipropyl	182	C6H14S3	006028-61-1	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011323\
Data File : VU052680.D
Acq On : 13 Jan 2023 15:27
Operator : JC/MD
Sample : 01139-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH1Y7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR011023WMA.M
Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Butanol	6.633	5.0	ug/L	41152900	1	6.247	41152900	5.0
Butanoic acid, ...	8.571	26.6	ug/L	2719070	2	9.414	511939	5.0
Acetic acid, bu...	8.829	16.8	ug/L	1719450	2	9.414	511939	5.0
Butanoic acid	9.276	15.6	ug/L	1595480	2	9.414	511939	5.0
Diethyl disulfide	10.575	17.3	ug/L	1773600	2	9.414	511939	5.0
Butanoic acid, ...	10.960	17.0	ug/L	1851990	3	11.809	543921	5.0
Ethanethioic ac...	11.153	11.9	ug/L	1292970	3	11.809	543921	5.0
Butanoic acid, ...	11.372	182.7	ug/L	19871600	3	11.809	543921	5.0
Ethyl n-butyl d...	12.999	6.6	ug/L	716564	3	11.809	543921	5.0
Butanethioic ac...	13.298	19.9	ug/L	2163740	3	11.809	543921	5.0
unknown-01	13.401	8.3	ug/L	900551	3	11.809	543921	5.0
unknown-02	15.398	7.2	ug/L	785786	3	11.809	543921	5.0