

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU091924\
 Data File : VU060912.D
 Acq On : 19 Sep 2024 20:45
 Operator : MD/SY
 Sample : P3987-18
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH8Q8

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: VU060912.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.660	408	426	489	rBV	1452224	7218565	24.17%	13.207%
2	2.952	507	517	568	rVB	309160	1010047	3.38%	1.848%
3	4.714	1026	1065	1144	rBV	8220819	29870266	100.00%	54.650%
4	5.062	1147	1173	1209	rBV4	593307	4606244	15.42%	8.427%
5	5.718	1358	1377	1392	rBV3	171749	440542	1.47%	0.806%
6	6.242	1530	1540	1573	rVB	175440	357854	1.20%	0.655%
7	6.386	1574	1585	1618	rVB	178329	370684	1.24%	0.678%
8	6.534	1618	1631	1643	rBV	156401	305589	1.02%	0.559%
9	6.763	1689	1702	1746	rVB	2007902	4460350	14.93%	8.161%
10	7.174	1802	1830	1872	rBV2	1239763	2962204	9.92%	5.420%
11	7.673	1972	1985	2019	rBV	173679	487843	1.63%	0.893%
12	7.891	2041	2053	2068	rVB	218506	395795	1.33%	0.724%
13	8.627	2273	2282	2309	rVB	194428	385869	1.29%	0.706%
14	9.412	2514	2526	2551	rVB	248764	420603	1.41%	0.770%
15	10.451	2838	2849	2871	rBV	206301	319520	1.07%	0.585%
16	11.361	3118	3132	3152	rBV2	161747	330198	1.11%	0.604%
17	11.804	3259	3270	3292	rVB	239794	394336	1.32%	0.721%
18	12.187	3375	3389	3410	rVB	191503	321078	1.07%	0.587%

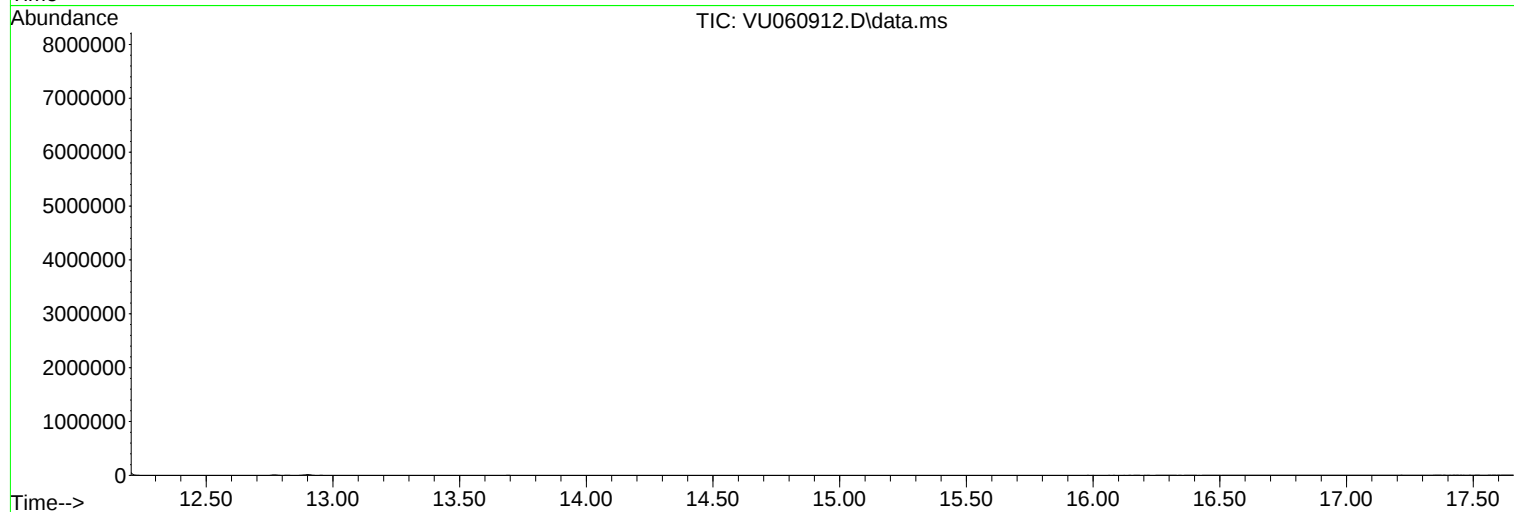
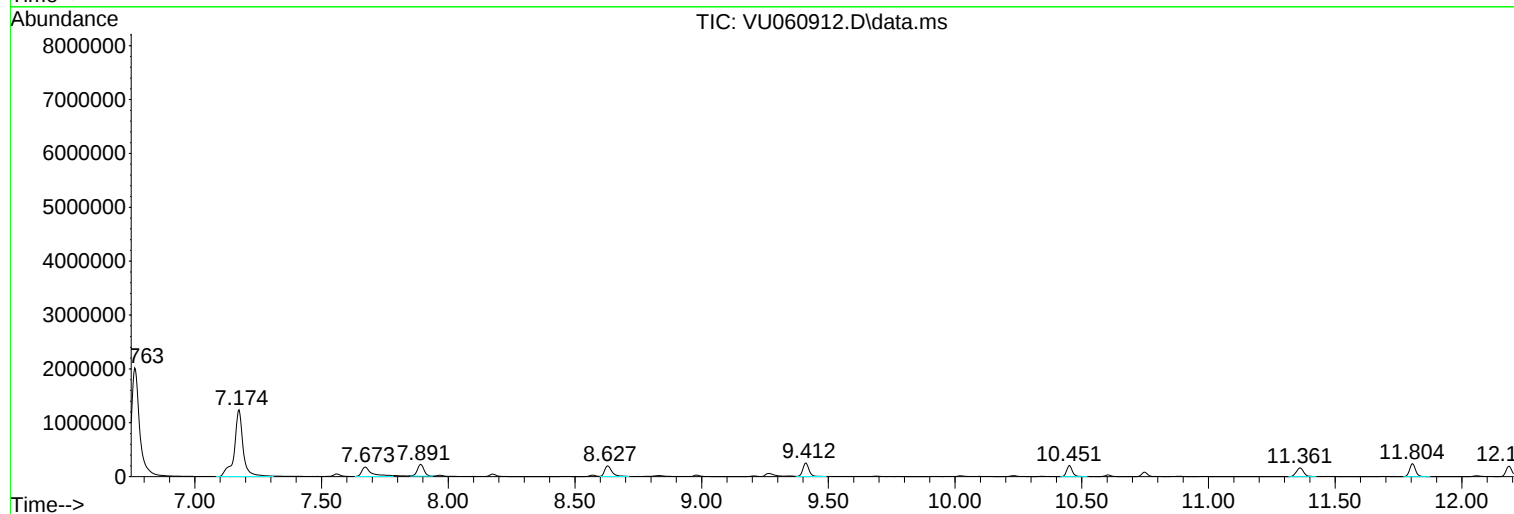
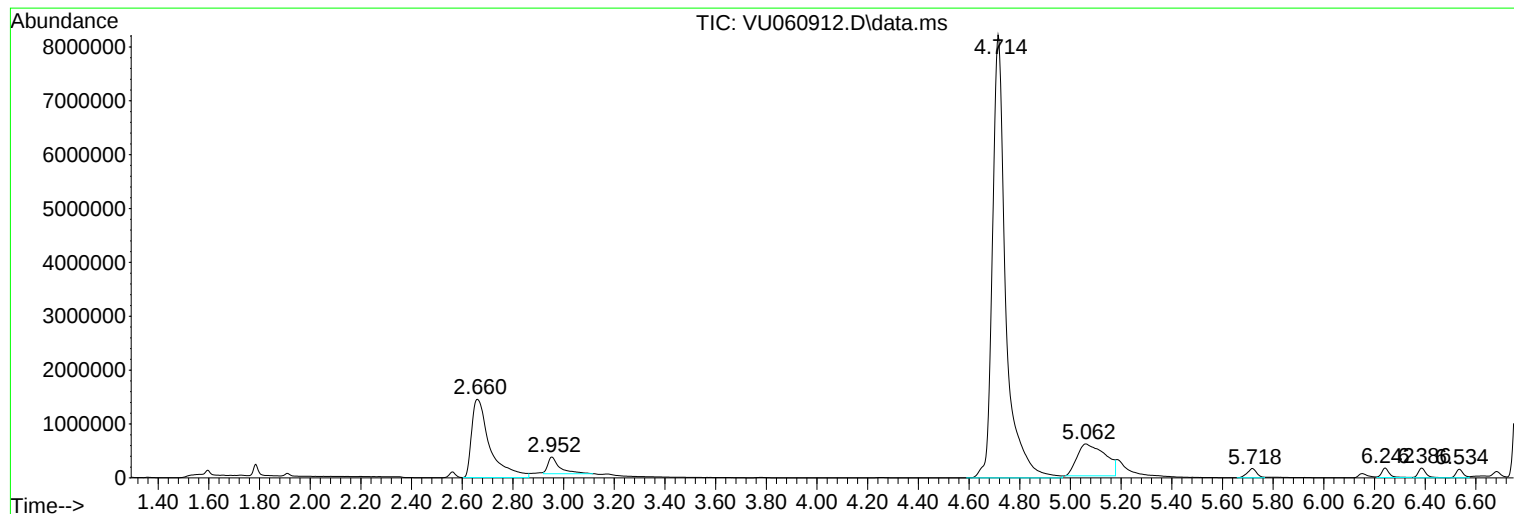
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091624WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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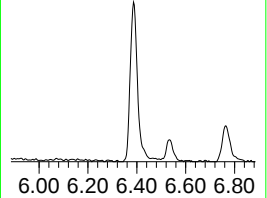
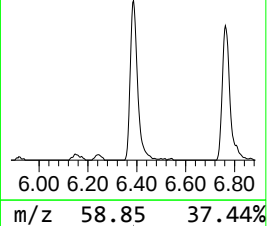
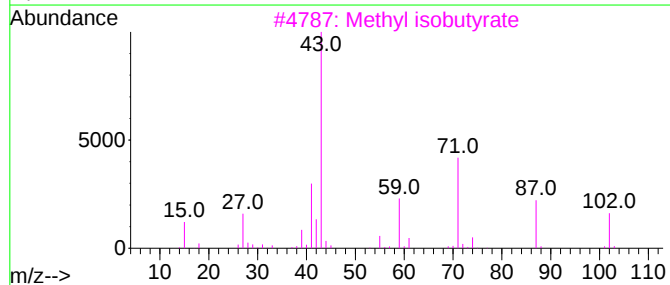
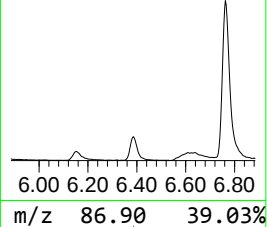
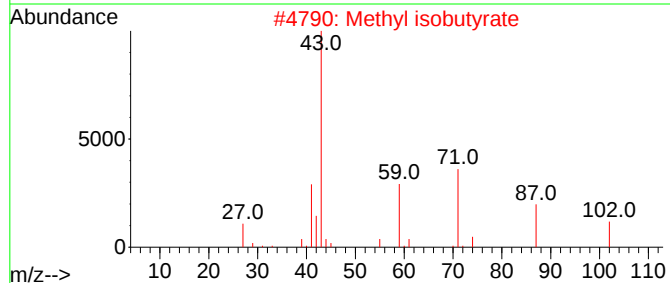
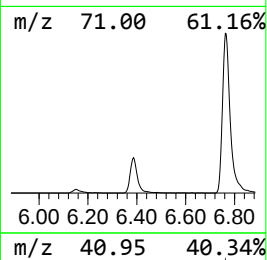
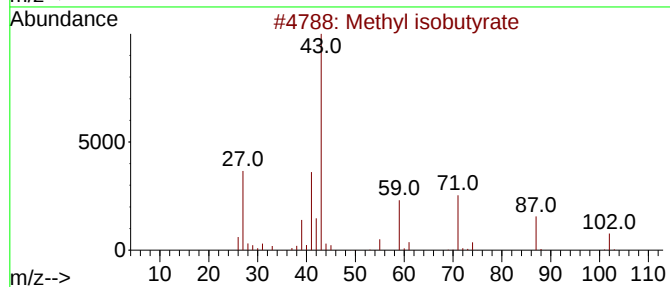
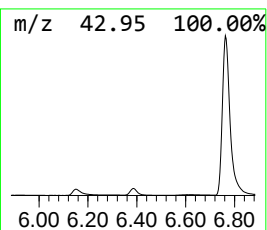
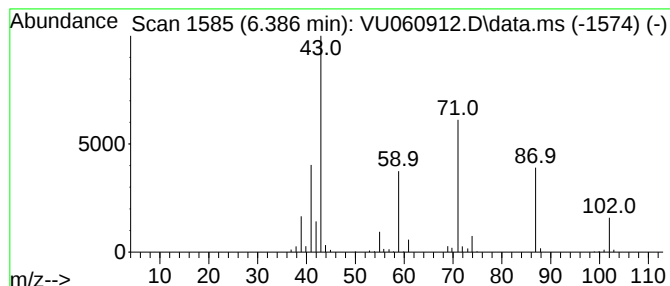
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Methyl isobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.386	5.18 ug/L	370684	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl isobutyrate	102	C5H10O2	000547-63-7	91
2			Methyl isobutyrate	102	C5H10O2	000547-63-7	90
3			Methyl isobutyrate	102	C5H10O2	000547-63-7	72
4			Methyl isobutyrate	102	C5H10O2	000547-63-7	64
5			Butyric acid hydrazide	102	C4H10N2O	003538-65-6	35



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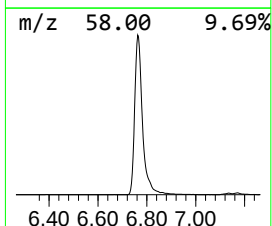
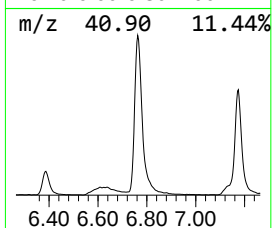
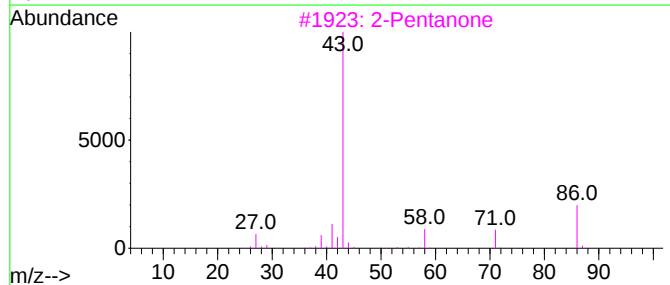
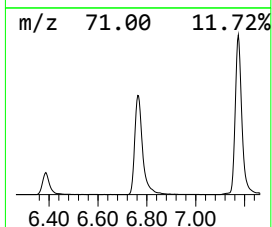
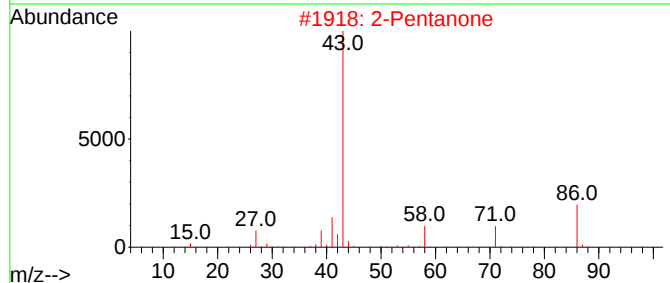
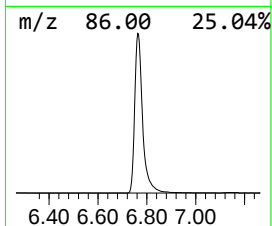
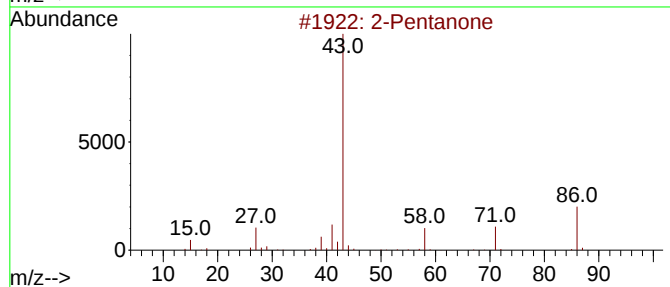
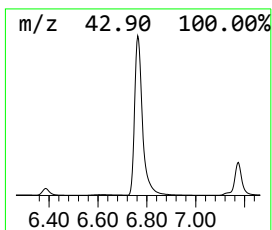
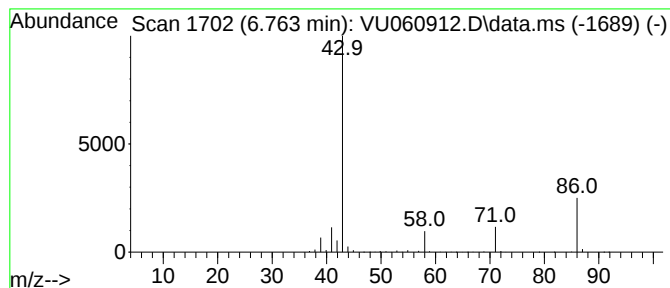
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091624WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 2-Pentanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.763	62.32 ug/L	4460350	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone			86	C5H10O	000107-87-9	90
2	2-Pentanone			86	C5H10O	000107-87-9	90
3	2-Pentanone			86	C5H10O	000107-87-9	87
4	2-Pentanone			86	C5H10O	000107-87-9	72
5	2-Butanone, 3-methyl-			86	C5H10O	000563-80-4	45



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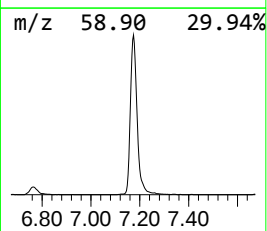
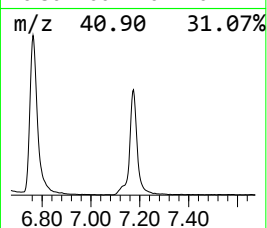
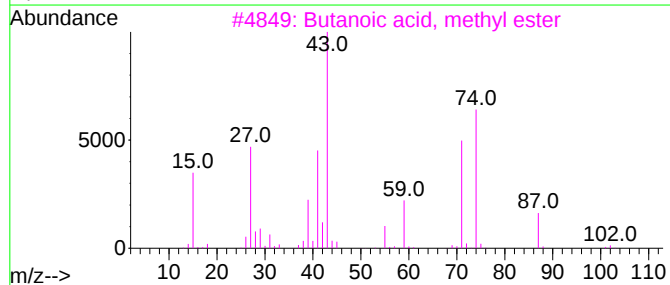
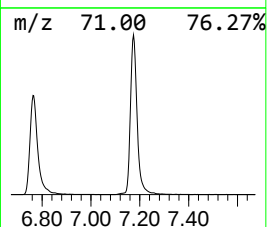
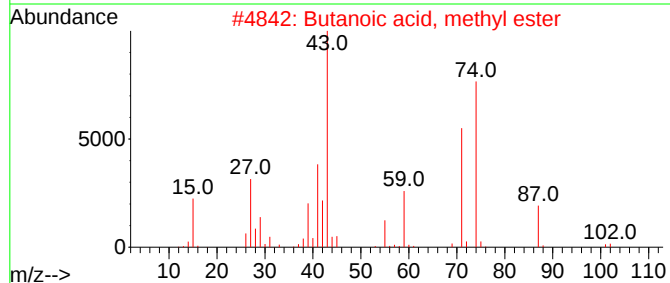
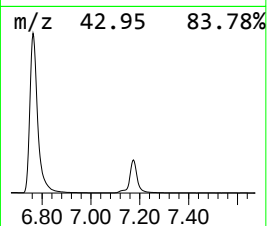
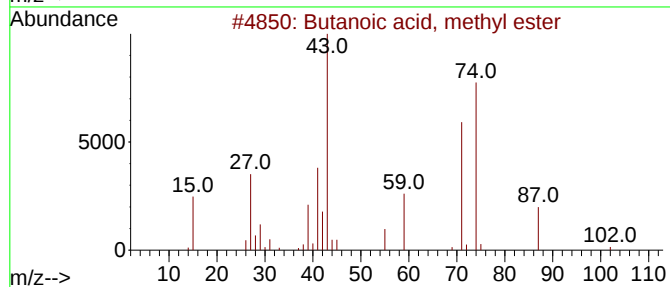
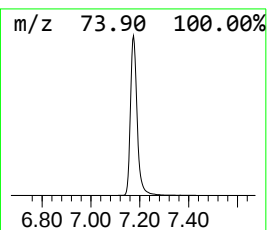
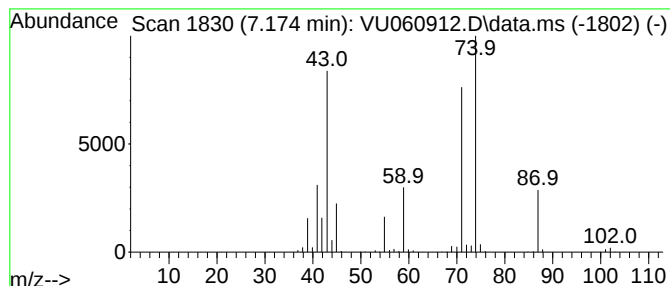
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Butanoic acid, methyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.174	41.39 ug/L	2962200	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	90
2			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	90
3			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	72
4			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	64
5			Pentane, 2-bromo-	150	C5H11Br	000107-81-3	27



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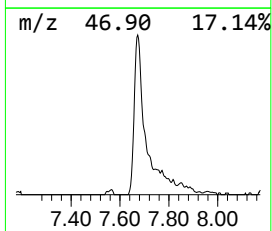
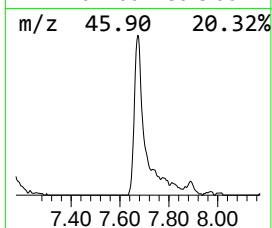
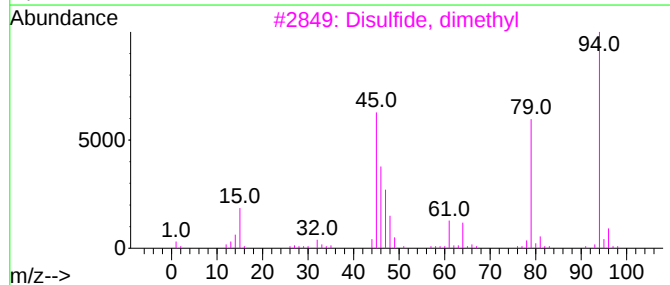
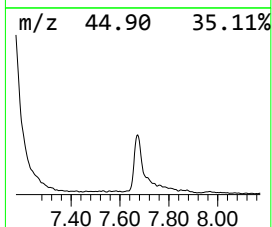
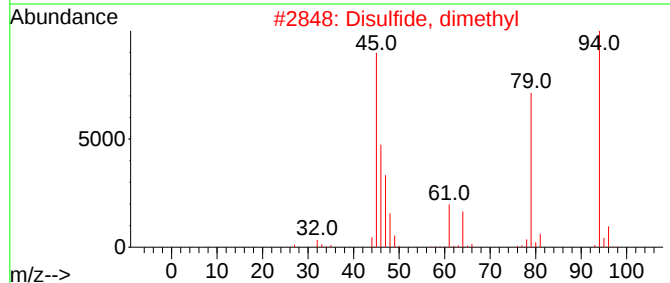
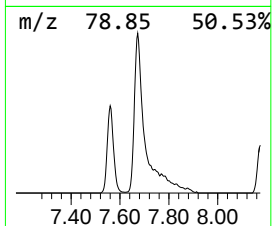
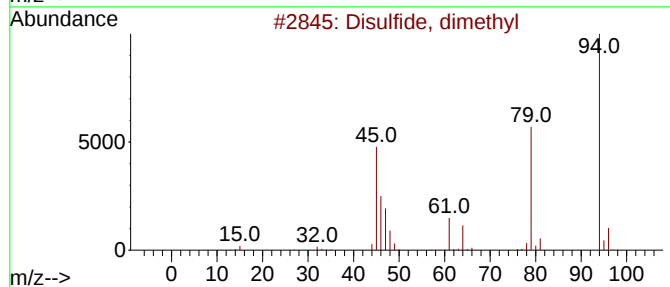
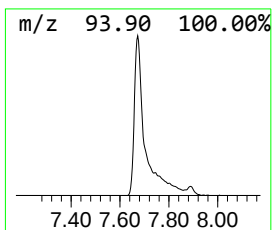
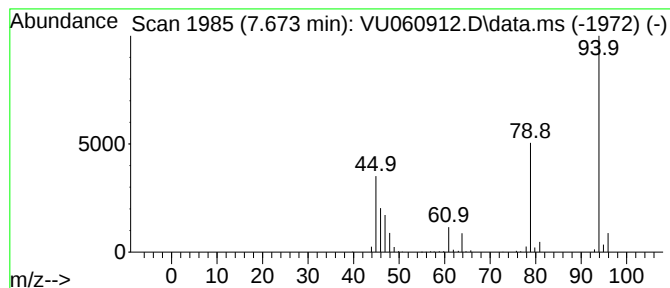
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Disulfide, dimethyl Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.673	6.82 ug/L	487843	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disulfide, dimethyl	94	C2H6S2	000624-92-0	96
2			Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
3			Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
4			Disulfide, dimethyl	94	C2H6S2	000624-92-0	91
5			Disulfide, dimethyl	94	C2H6S2	000624-92-0	91



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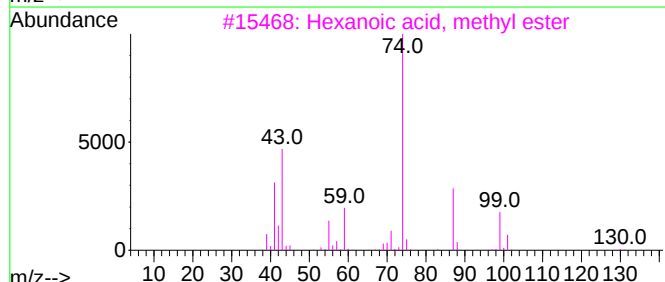
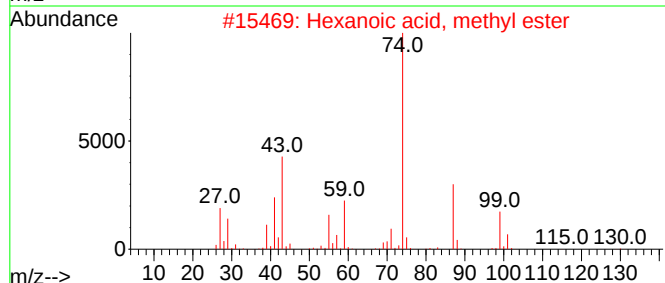
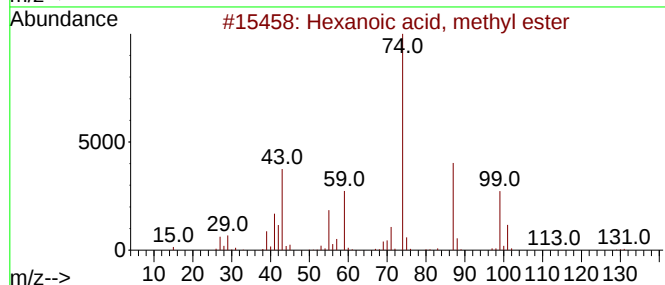
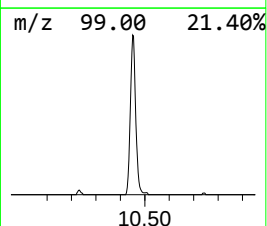
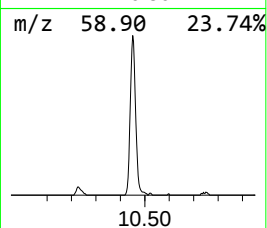
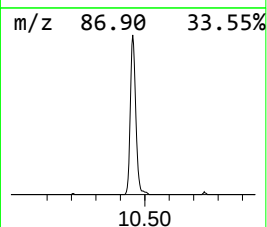
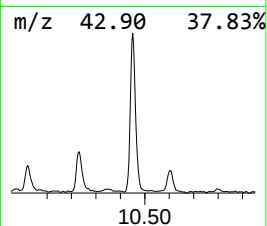
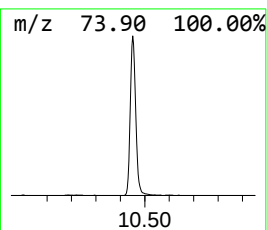
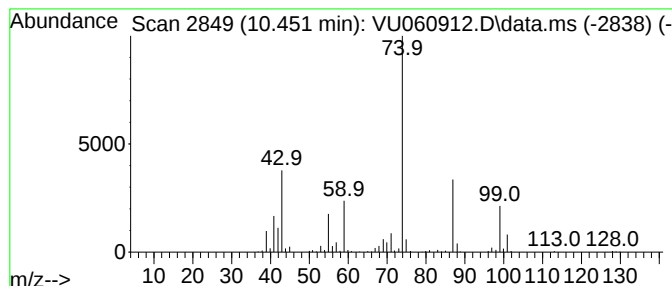
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Hexanoic acid, methyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.451	3.80 ug/L	319520	Chlorobenzene-d5	9.412

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	92
2			Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	90
3			Hexanoic acid, methyl ester	130	C7H14O2	000106-70-7	90
4			Methyl valerate	116	C6H12O2	000624-24-8	59
5			Heptanoic acid, methyl ester	144	C8H16O2	000106-73-0	53



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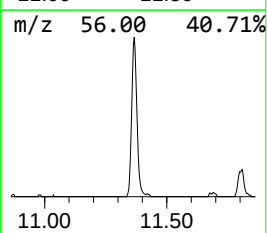
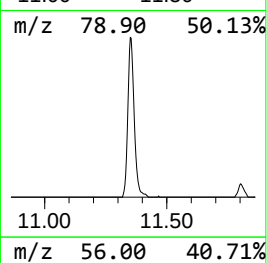
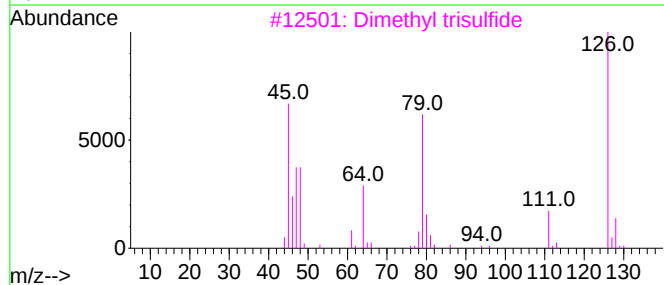
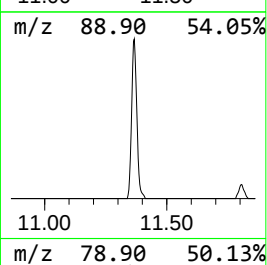
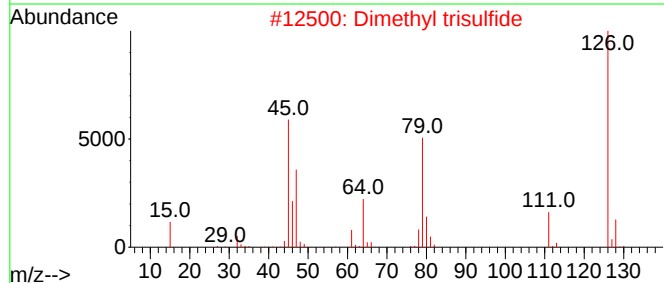
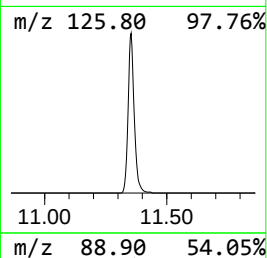
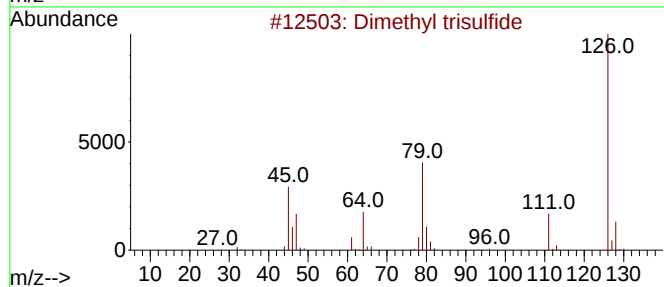
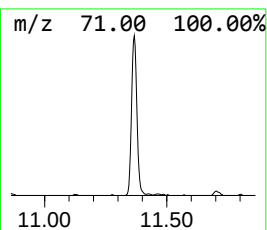
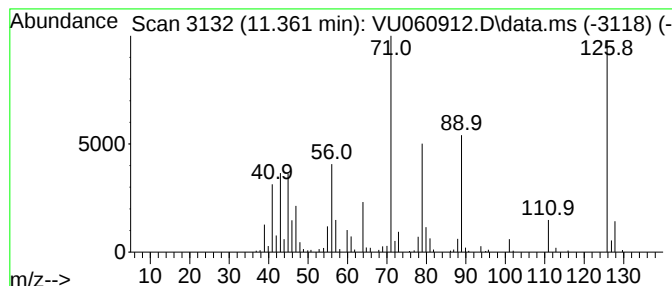
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR091624WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Dimethyl trisulfide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.361	4.19 ug/L	330198	1,4-Dichlorobenzene-d4	11.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl trisulfide	126	C2H6S3	003658-80-8	89
2			Dimethyl trisulfide	126	C2H6S3	003658-80-8	64
3			Dimethyl trisulfide	126	C2H6S3	003658-80-8	50
4			Dimethyl trisulfide	126	C2H6S3	003658-80-8	38
5			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU091924\
Data File : VU060912.D
Acq On : 19 Sep 2024 20:45
Operator : MD/SY
Sample : P3987-18
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH8Q8

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methyl isobutyrate	6.386	5.2	ug/L	370684	1	6.242	357854	5.0
2-Pentanone	6.763	62.3	ug/L	4460350	1	6.242	357854	5.0
Butanoic acid, ...	7.174	41.4	ug/L	2962200	1	6.242	357854	5.0
Disulfide, dime...	7.673	6.8	ug/L	487843	1	6.242	357854	5.0
Hexanoic acid, ...	10.451	3.8	ug/L	319520	2	9.412	420603	5.0
Dimethyl trisul...	11.361	4.2	ug/L	330198	3	11.804	394336	5.0