

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV091824\
 Data File : VV037360.D
 Acq On : 19 Sep 2024 02:43
 Operator : SY/MD
 Sample : P3986-04
 Misc : 25mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BH8M4

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_V\Method\SFAMVTR091024WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VV037360.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.307	67	83	95	rBV2	332329	404636	3.23%	1.163%
2	1.471	125	134	152	rBV	677446	1076978	8.59%	3.097%
3	1.577	161	167	192	rVB3	185187	333578	2.66%	0.959%
4	1.802	229	237	243	rBV	102635	181108	1.44%	0.521%
5	2.102	321	330	342	rBV3	432889	743773	5.93%	2.139%
6	3.172	653	663	677	rVB	150612	315058	2.51%	0.906%
7	3.886	867	885	897	rBV	1565413	4125781	32.90%	11.863%
8	4.995	1219	1230	1249	rVB2	466438	1016885	8.11%	2.924%
9	5.545	1391	1401	1422	rVB	347579	672142	5.36%	1.933%
10	5.738	1452	1461	1473	rBV	76368	154800	1.23%	0.445%
11	5.818	1475	1486	1497	rBV	715024	1325306	10.57%	3.811%
12	6.130	1575	1583	1608	rVB2	1121908	2762317	22.03%	7.943%
13	6.558	1700	1716	1774	rVB2	5056033	12540420	100.00%	36.058%
14	6.912	1819	1826	1835	rBV2	216123	293936	2.34%	0.845%
15	7.285	1934	1942	1950	rBV	561851	1004495	8.01%	2.888%
16	8.011	2161	2168	2177	rBV	535133	796290	6.35%	2.290%
17	8.072	2179	2187	2211	rVB	562655	1060606	8.46%	3.050%
18	8.275	2243	2250	2259	rBV	337642	529466	4.22%	1.522%
19	10.156	2828	2835	2847	rVB	199048	315371	2.51%	0.907%
20	10.789	3023	3032	3051	rBV	623756	917553	7.32%	2.638%
21	11.182	3145	3154	3164	rBV	615200	965853	7.70%	2.777%
22	11.471	3234	3244	3260	rBV	802180	1253825	10.00%	3.605%
23	11.555	3262	3270	3288	rVB	495644	776555	6.19%	2.233%
24	12.172	3454	3462	3470	rBV	369105	535016	4.27%	1.538%
25	12.220	3470	3477	3491	rVB	461826	676333	5.39%	1.945%

Sum of corrected areas: 34778081

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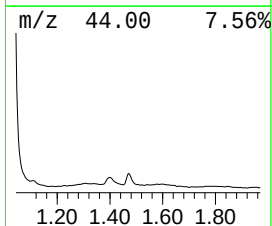
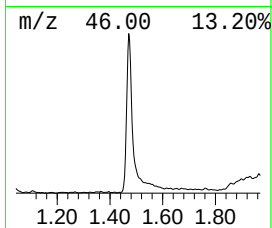
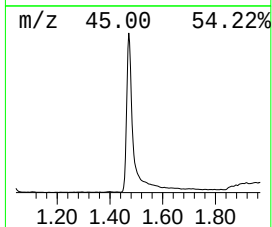
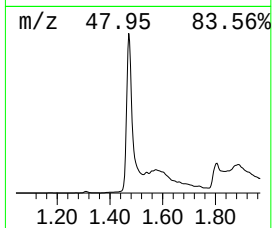
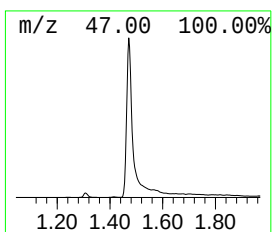
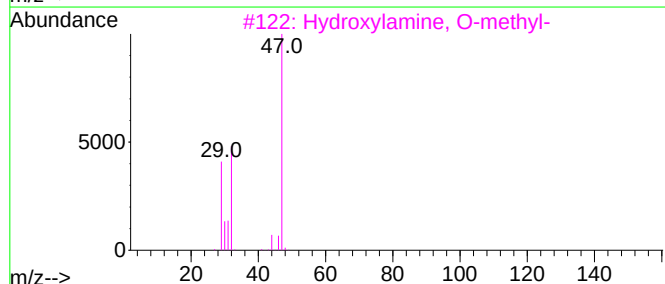
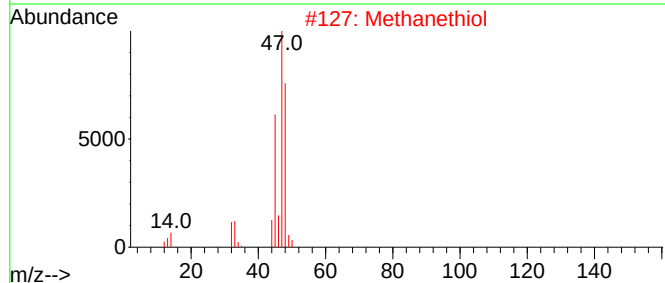
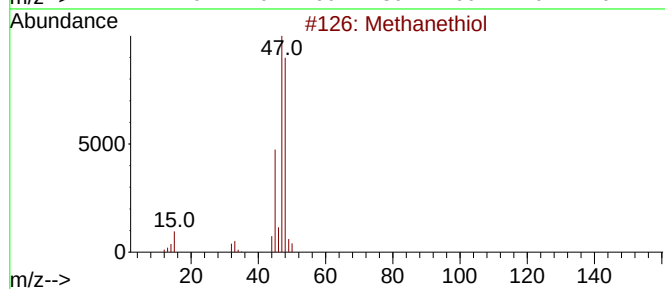
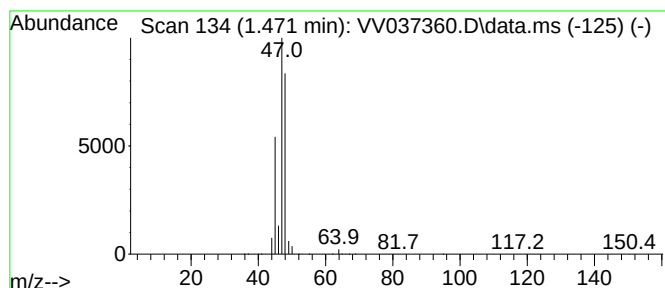
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Methanethiol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.471	8.01 ug/L	1076980	1,4-Difluorobenzene	5.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanethiol	48	CH4S	000074-93-1	90
2			Methanethiol	48	CH4S	000074-93-1	83
3			Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
4			Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
5			Methane, nitroso-	45	CH3NO	000865-40-7	5



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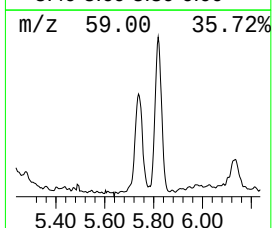
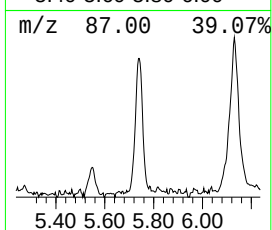
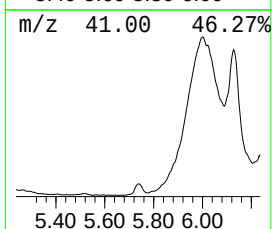
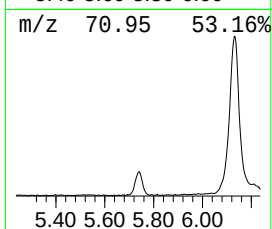
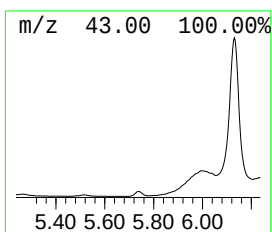
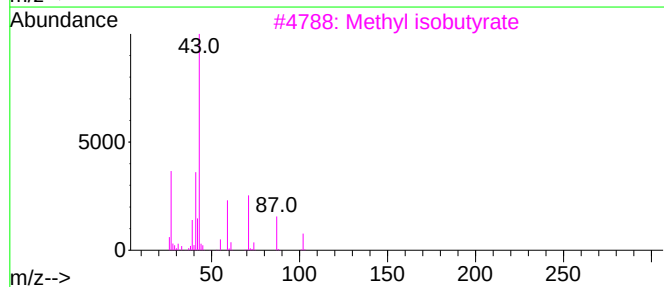
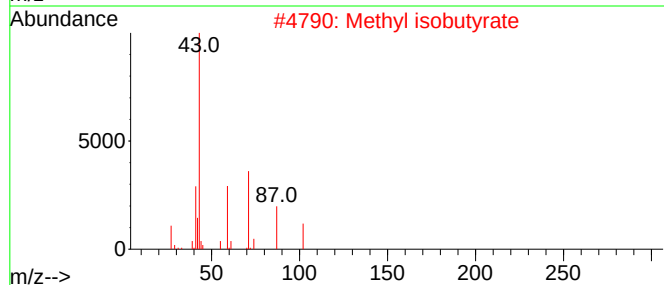
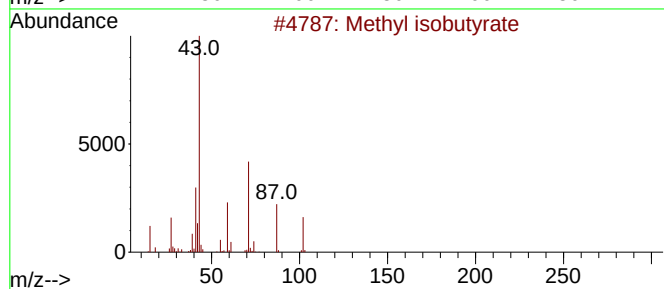
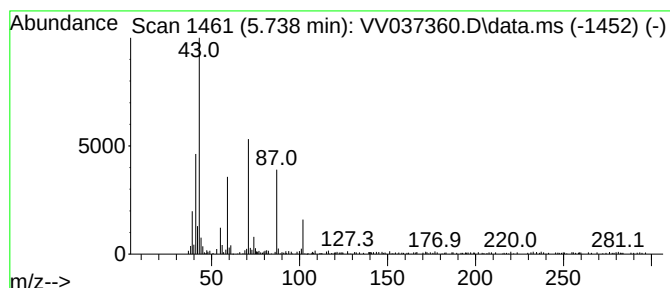
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Methyl isobutyrate Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.738	1.15 ug/L	154800	1,4-Difluorobenzene	5.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl isobutyrate	102	C5H10O2	000547-63-7	58
2			Methyl isobutyrate	102	C5H10O2	000547-63-7	53
3			Methyl isobutyrate	102	C5H10O2	000547-63-7	53
4			Methyl isobutyrate	102	C5H10O2	000547-63-7	49
5			Butyric acid hydrazide	102	C4H10N2O	003538-65-6	35



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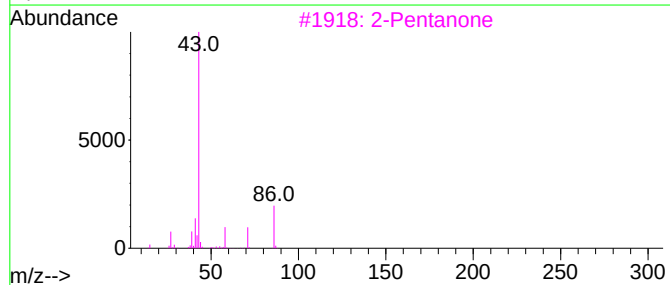
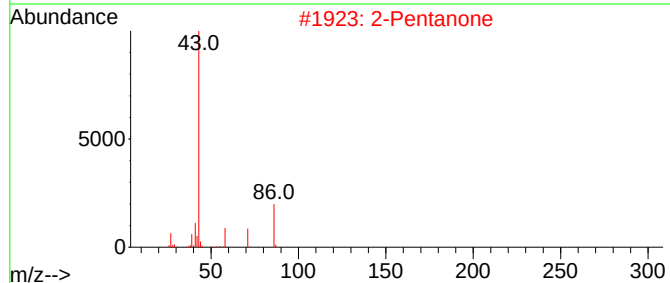
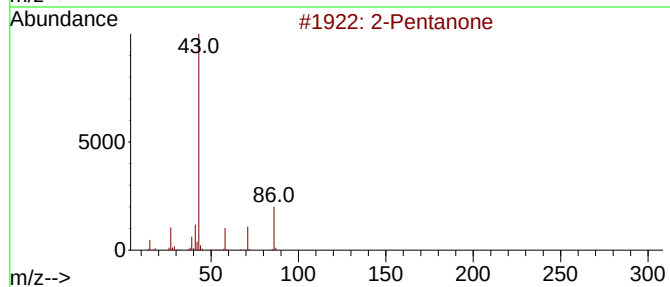
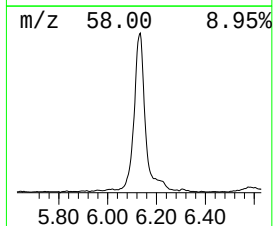
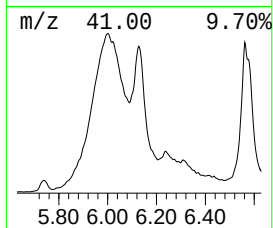
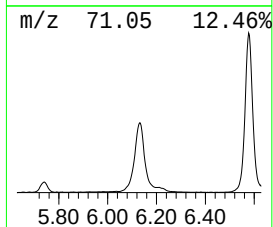
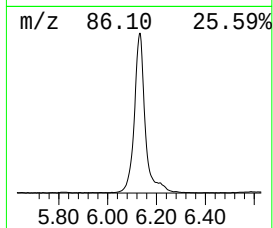
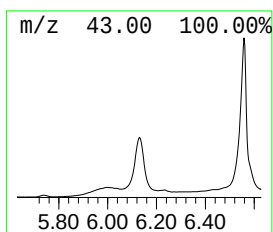
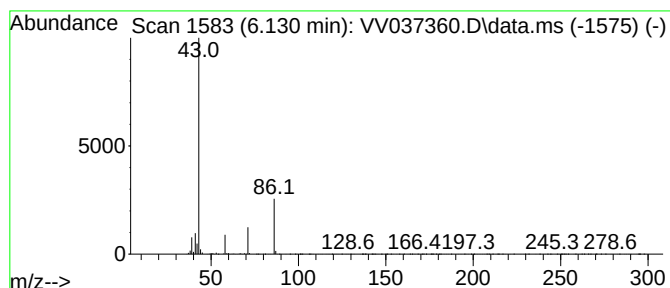
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR091024WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 2-Pentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.130	20.55 ug/L	2762320	1,4-Difluorobenzene	5.545

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	86
3	2-Pentanone			86	C5H10O	000107-87-9	86
4	2-Butanone, 3-methyl-			86	C5H10O	000563-80-4	64
5	1-Butanol, 2-methylene-, acetate			128	C7H12O2	055670-09-2	9



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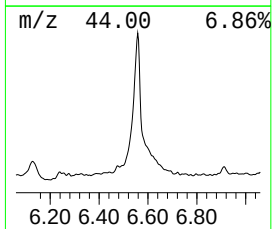
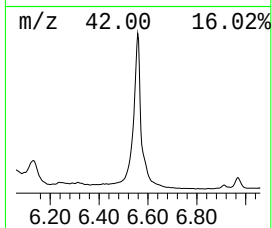
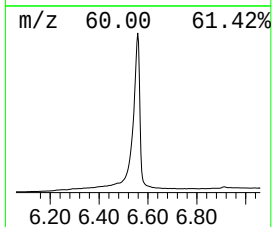
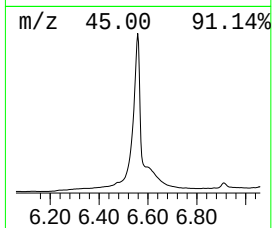
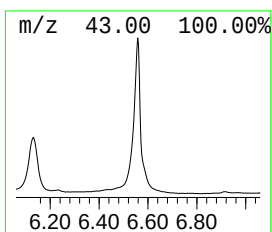
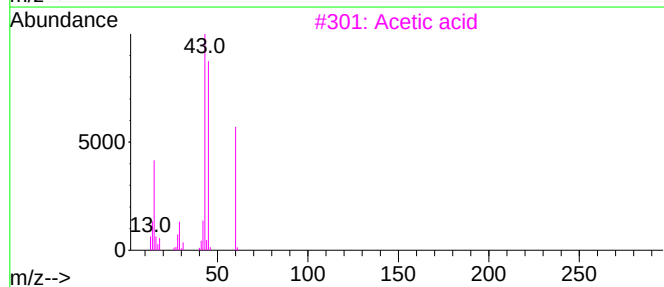
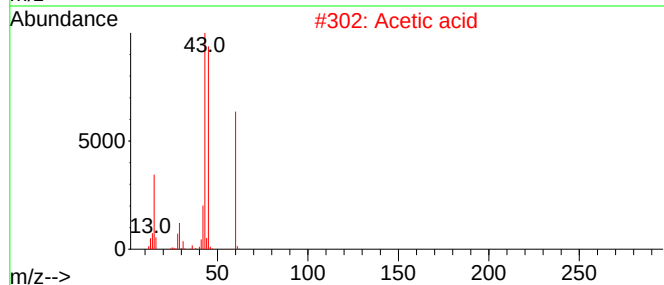
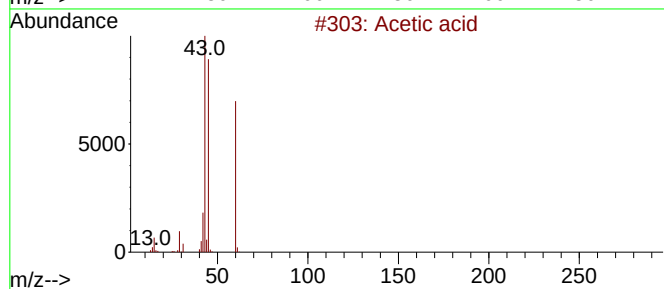
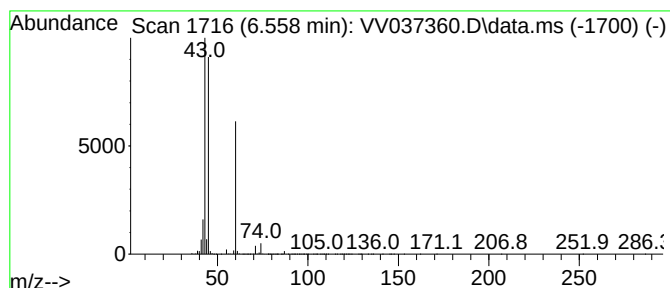
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Acetic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.558	93.29 ug/L	12540400	1,4-Difluorobenzene	5.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid			60	C2H4O2	000064-19-7	87
2	Acetic acid			60	C2H4O2	000064-19-7	86
3	Acetic acid			60	C2H4O2	000064-19-7	86
4	Acetic acid			60	C2H4O2	000064-19-7	78
5	Acetic acid			60	C2H4O2	000064-19-7	78



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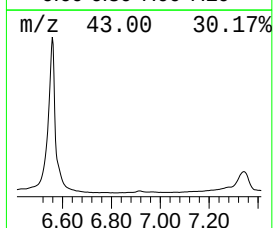
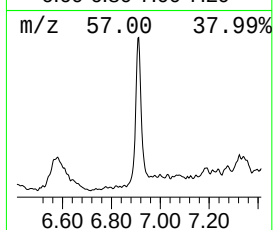
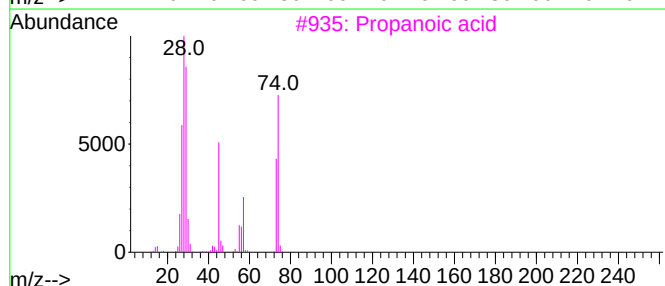
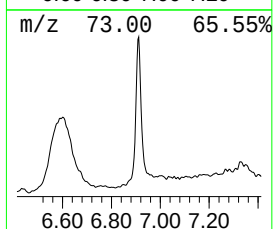
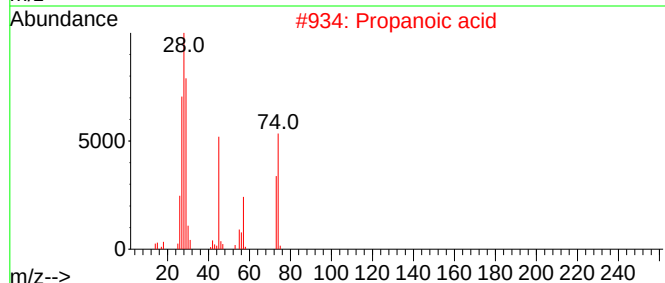
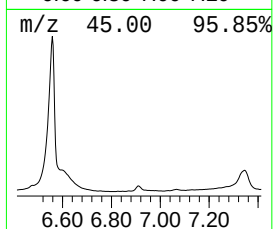
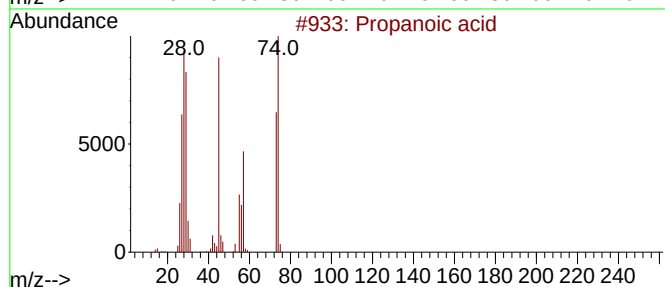
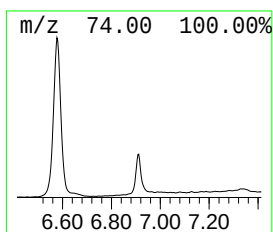
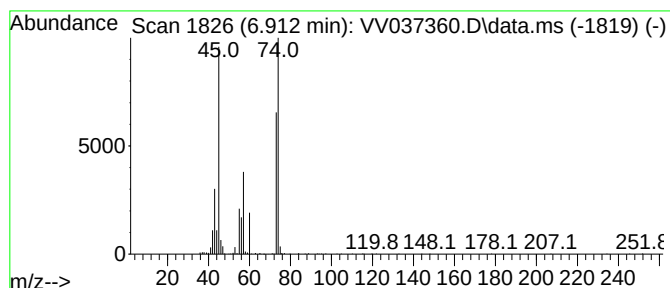
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Propanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.912	2.19 ug/L	293936	1,4-Difluorobenzene	5.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid			74	C3H6O2	000079-09-4	87
2	Propanoic acid			74	C3H6O2	000079-09-4	83
3	Propanoic acid			74	C3H6O2	000079-09-4	52
4	Propanoic acid			74	C3H6O2	000079-09-4	52
5	Propanoic acid			74	C3H6O2	000079-09-4	50



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Quant Title : TRACE VOA SFAM1.0

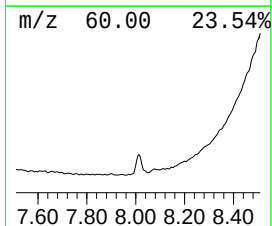
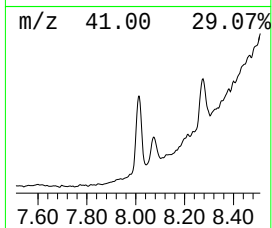
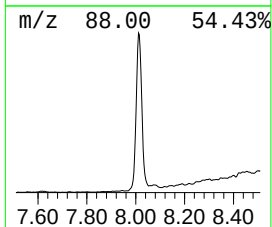
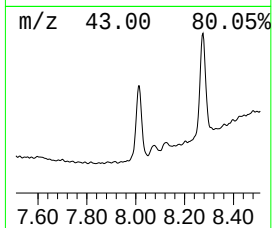
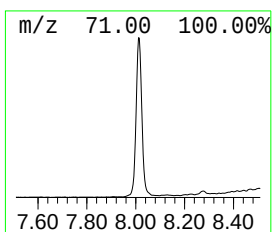
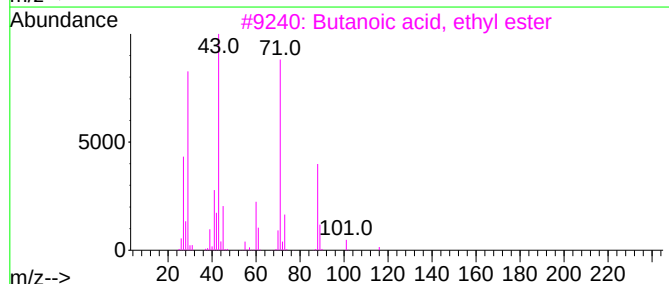
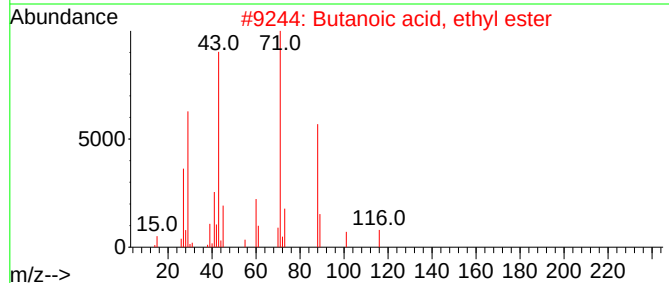
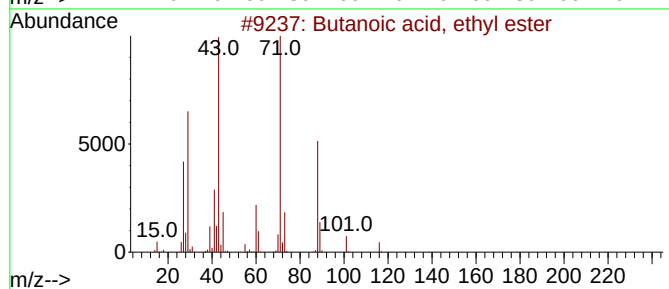
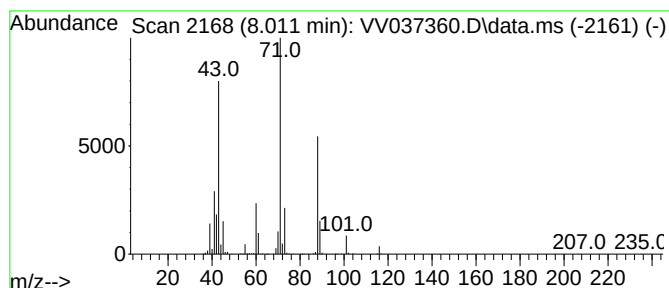
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Butanoic acid, ethyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.011	7.52 ug/L	796290	Chlorobenzene-d5	8.799

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	86
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	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV091824\
Data File : VV037360.D
Acq On : 19 Sep 2024 02:43
Operator : SY/MD
Sample : P3986-04
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8M4

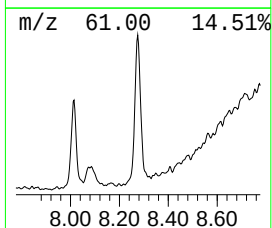
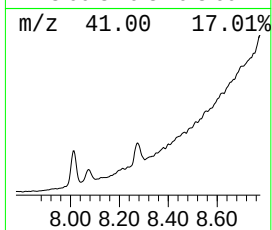
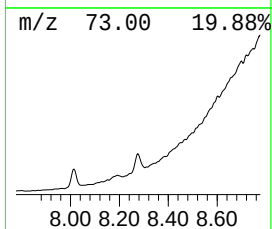
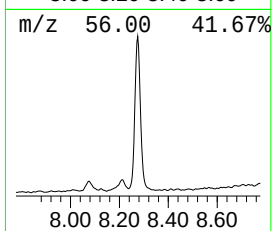
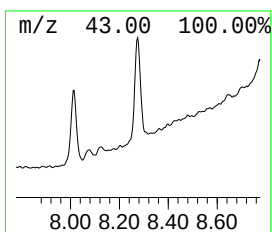
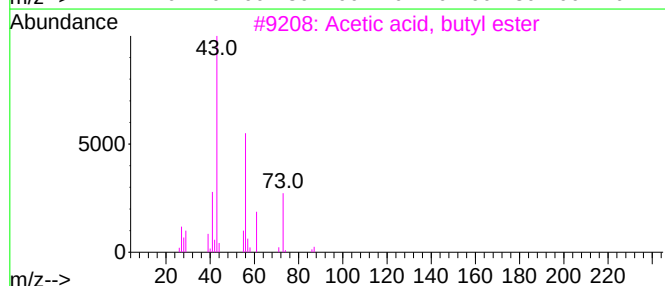
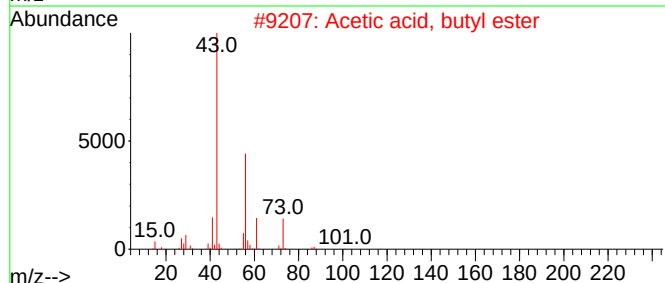
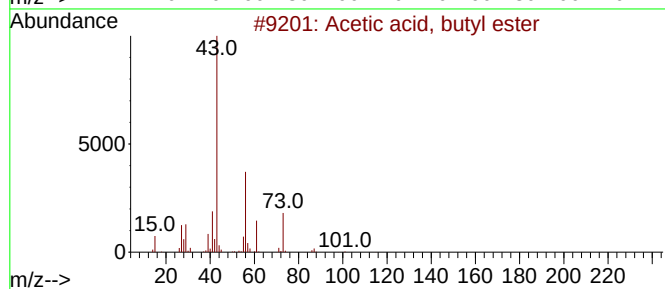
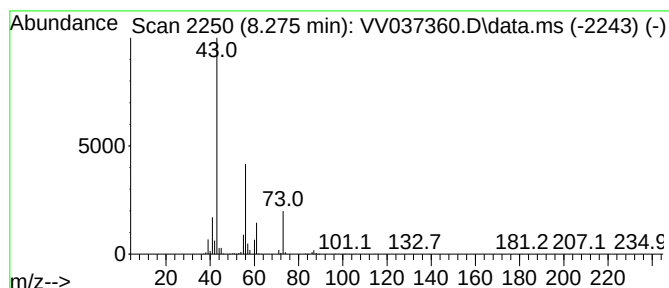
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 Acetic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.275	5.00 ug/L	529466	Chlorobenzene-d5	8.799

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester		116	C6H12O2		000123-86-4	78
2	Acetic acid, butyl ester		116	C6H12O2		000123-86-4	78
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	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV091824\
Data File : VV037360.D
Acq On : 19 Sep 2024 02:43
Operator : SY/MD
Sample : P3986-04
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8M4

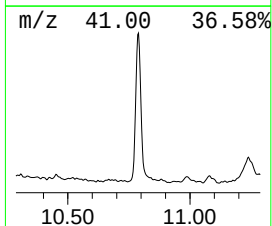
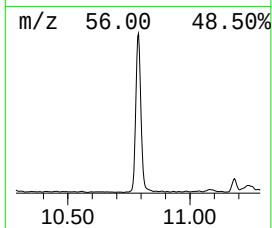
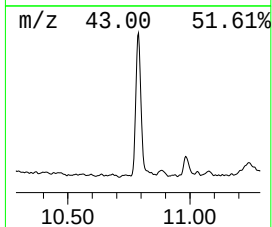
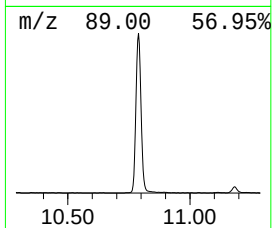
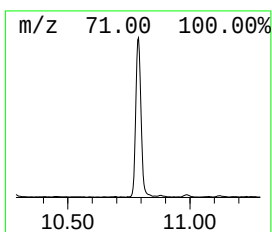
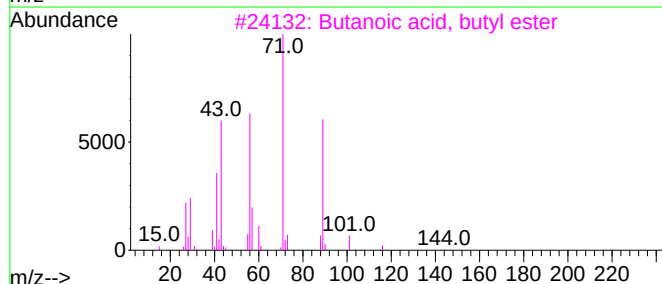
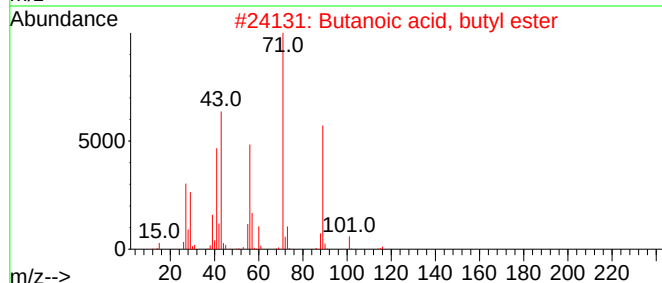
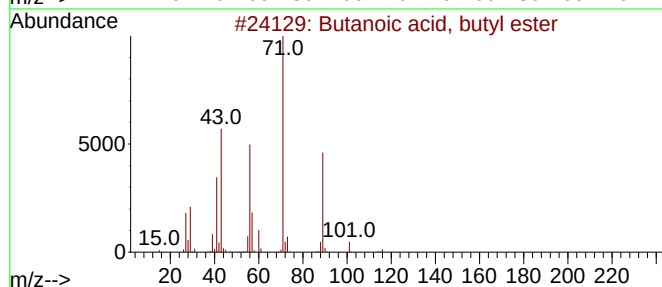
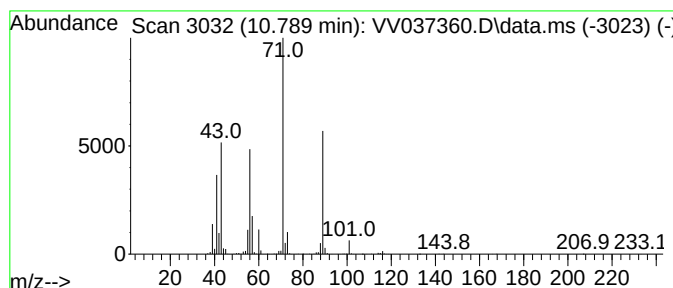
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 Butanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.789	4.75 ug/L	917553	1,4-Dichlorobenzene-d4	11.182

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, butyl ester	144	C8H16O2	000109-21-7	90
4			Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72
5			Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV091824\
Data File : VV037360.D
Acq On : 19 Sep 2024 02:43
Operator : SY/MD
Sample : P3986-04
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8M4

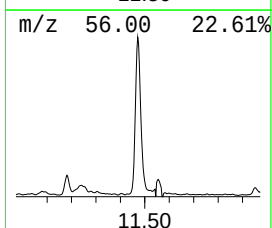
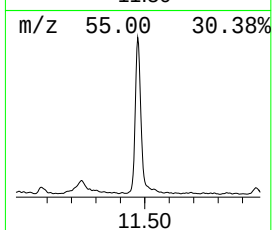
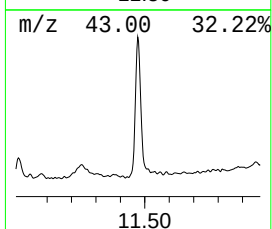
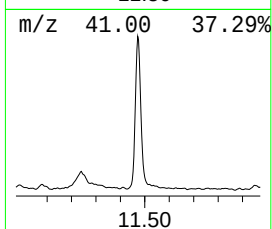
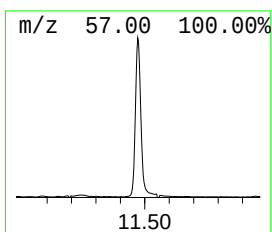
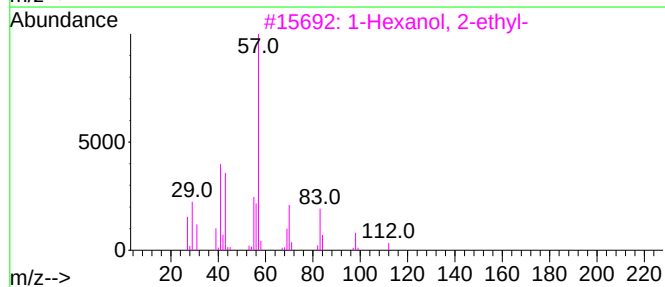
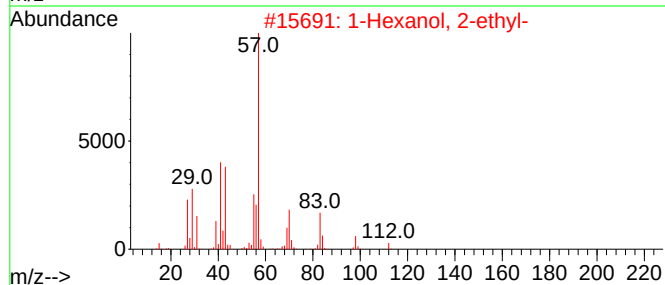
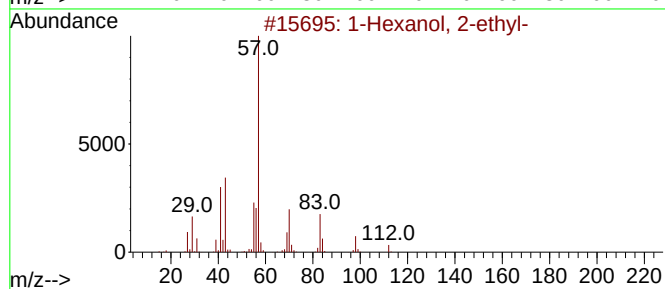
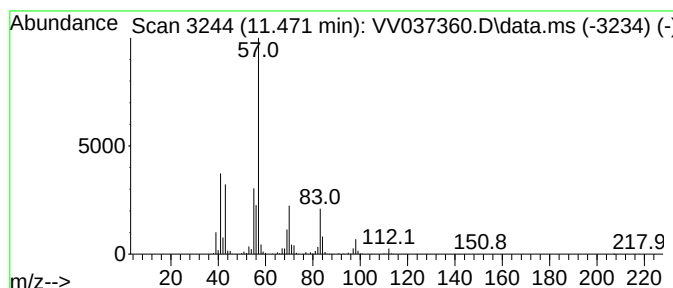
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.471	6.49 ug/L	1253830	1,4-Dichlorobenzene-d4	11.182

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
3		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
4		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
5		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV091824\
Data File : VV037360.D
Acq On : 19 Sep 2024 02:43
Operator : SY/MD
Sample : P3986-04
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

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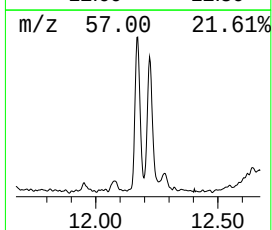
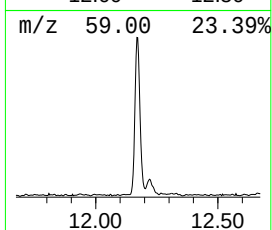
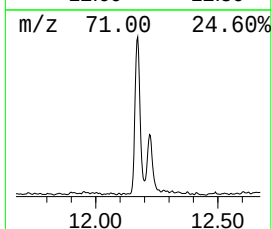
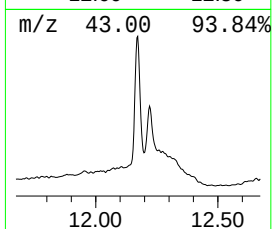
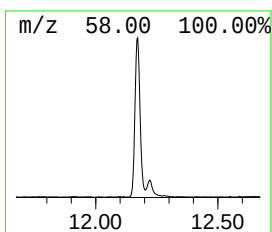
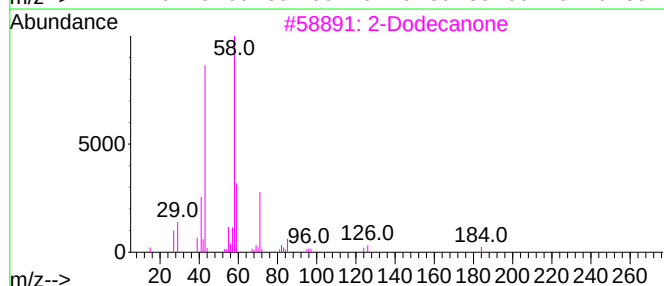
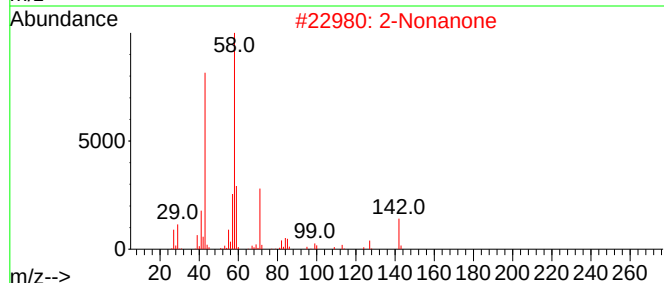
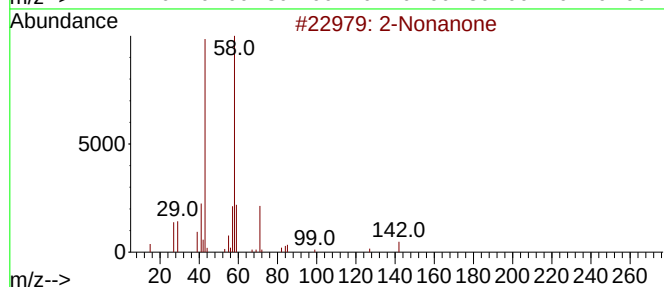
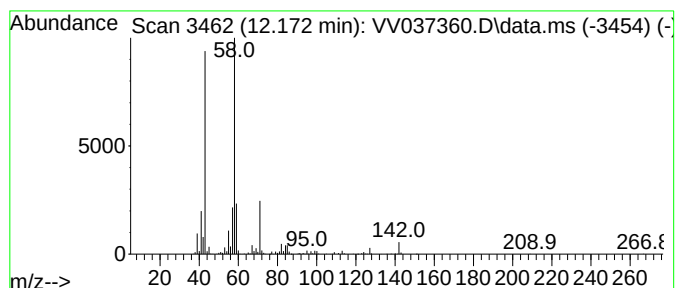
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 11 2-Nonanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.172	2.77 ug/L	535016	1,4-Dichlorobenzene-d4	11.182

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Nonanone	142	C9H18O	000821-55-6	94
2		2-Nonanone	142	C9H18O	000821-55-6	91
3		2-Dodecanone	184	C12H24O	006175-49-1	78
4		2,4(3H,5H)-Furandione, 5-hexyl-5...	198	C11H18O3	054852-79-8	64
5		2-Undecanone	170	C11H22O	000112-12-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV091824\
Data File : VV037360.D
Acq On : 19 Sep 2024 02:43
Operator : SY/MD
Sample : P3986-04
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8M4

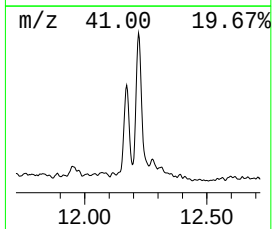
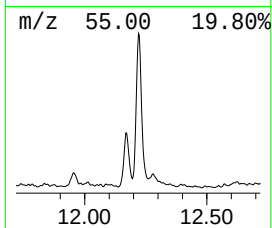
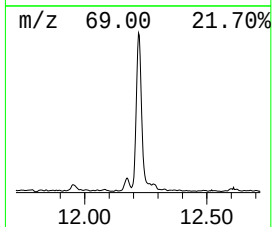
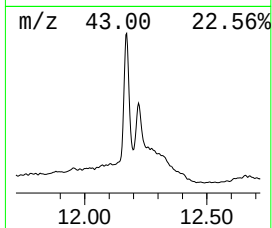
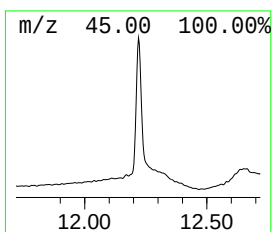
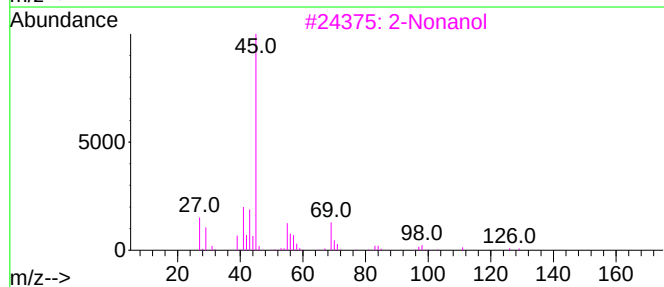
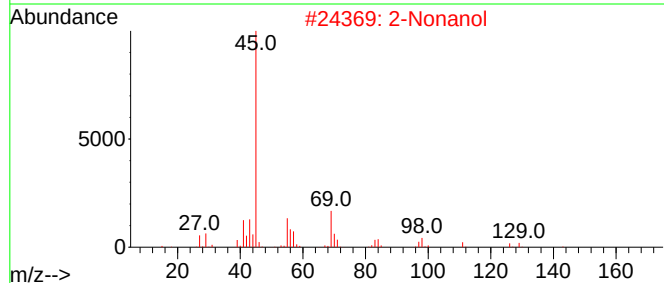
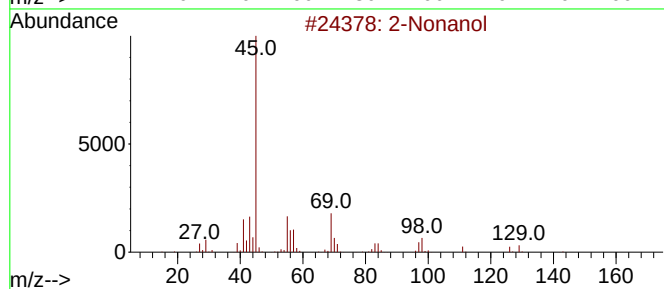
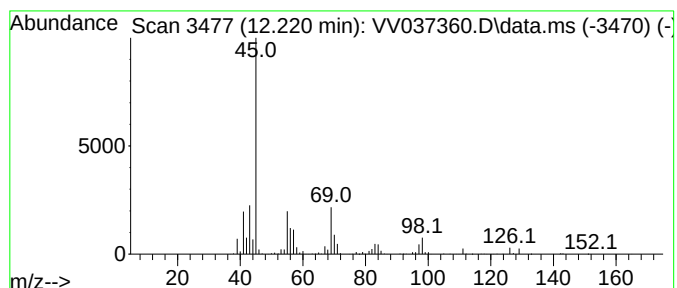
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 12 2-Nonanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.220	3.50 ug/L	676333	1,4-Dichlorobenzene-d4	11.182

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Nonanol	144	C9H20O	000628-99-9	90
2		2-Nonanol	144	C9H20O	000628-99-9	90
3		2-Nonanol	144	C9H20O	000628-99-9	83
4		2-Undecanol	172	C11H24O	001653-30-1	78
5		2-Decanol	158	C10H22O	001120-06-5	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV091824\
Data File : VV037360.D
Acq On : 19 Sep 2024 02:43
Operator : SY/MD
Sample : P3986-04
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8M4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR091024WMA.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
Methanethiol	1.471	8.0	ug/L	1076980	1	5.545	672142	5.0
Methyl isobutyrate	5.738	1.1	ug/L	154800	1	5.545	672142	5.0
2-Pentanone	6.130	20.6	ug/L	2762320	1	5.545	672142	5.0
Acetic acid	6.558	93.3	ug/L	12540400	1	5.545	672142	5.0
Propanoic acid	6.912	2.2	ug/L	293936	1	5.545	672142	5.0
Butanoic acid, ...	8.011	7.5	ug/L	796290	2	8.799	529466	5.0
Acetic acid, bu...	8.275	5.0	ug/L	529466	2	8.799	529466	5.0
Butanoic acid, ...	10.789	4.8	ug/L	917553	3	11.182	965853	5.0
1-Hexanol, 2-et...	11.471	6.5	ug/L	1253830	3	11.182	965853	5.0
2-Nonanone	12.172	2.8	ug/L	535016	3	11.182	965853	5.0
2-Nonanol	12.220	3.5	ug/L	676333	3	11.182	965853	5.0