

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV091924\
 Data File : VV037404.D
 Acq On : 20 Sep 2024 00:42
 Operator : SY/MD
 Sample : P3988-14 20X
 Misc : 25mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BH8S3

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: VV037404.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.275	60	73	84	rBV2	155654	208402	12.59%	1.508%
2	1.371	90	103	104	rBV3	52253	98388	5.94%	0.712%
3	1.429	116	121	133	rVB2	57309	78371	4.74%	0.567%
4	1.529	146	152	168	rVB	109742	143837	8.69%	1.041%
5	1.976	286	291	299	rVB	22908	29100	1.76%	0.211%
6	2.047	304	313	330	rVB	239199	377834	22.83%	2.733%
7	2.169	334	351	365	rBV3	73148	315167	19.04%	2.280%
8	2.548	462	469	494	rVB2	63885	154804	9.35%	1.120%
9	3.101	631	641	661	rVB2	13086	29083	1.76%	0.210%
10	3.600	777	796	798	rBV7	9669	22720	1.37%	0.164%
11	3.822	850	865	877	rBV4	136897	450459	27.22%	3.259%
12	4.240	980	995	1023	rVB	175768	469955	28.40%	3.400%
13	4.950	1199	1216	1250	rBV2	406300	1064889	64.34%	7.704%
14	5.529	1385	1396	1435	rBV	326347	726720	43.91%	5.257%
15	5.838	1481	1492	1512	rBV2	29024	72077	4.36%	0.521%
16	5.989	1526	1539	1548	rBV2	583354	1654972	100.00%	11.972%
17	6.294	1627	1634	1662	rVB2	69143	172923	10.45%	1.251%
18	6.911	1815	1826	1848	rBV	89889	184537	11.15%	1.335%
19	7.239	1917	1928	1957	rBV	435137	815766	49.29%	5.901%
20	7.558	2019	2027	2047	rBV2	49147	98329	5.94%	0.711%
21	7.972	2146	2156	2166	rBV	431723	719815	43.49%	5.207%
22	8.034	2166	2175	2203	rVB	521681	1193629	72.12%	8.635%
23	8.249	2234	2242	2265	rBV2	72648	151464	9.15%	1.096%
24	8.783	2396	2408	2433	rBV	507117	901566	54.48%	6.522%
25	9.079	2491	2500	2515	rBV3	22690	44862	2.71%	0.325%
26	9.490	2618	2628	2646	rBV	122346	235537	14.23%	1.704%
27	9.638	2665	2674	2697	rBV	65969	133523	8.07%	0.966%
28	10.152	2822	2834	2851	rBV	218281	362318	21.89%	2.621%
29	10.786	3021	3031	3066	rBV	719604	1169862	70.69%	8.463%
30	11.181	3143	3154	3176	rVV	566902	903999	54.62%	6.540%
31	11.558	3249	3271	3297	rBV	498808	838423	50.66%	6.065%

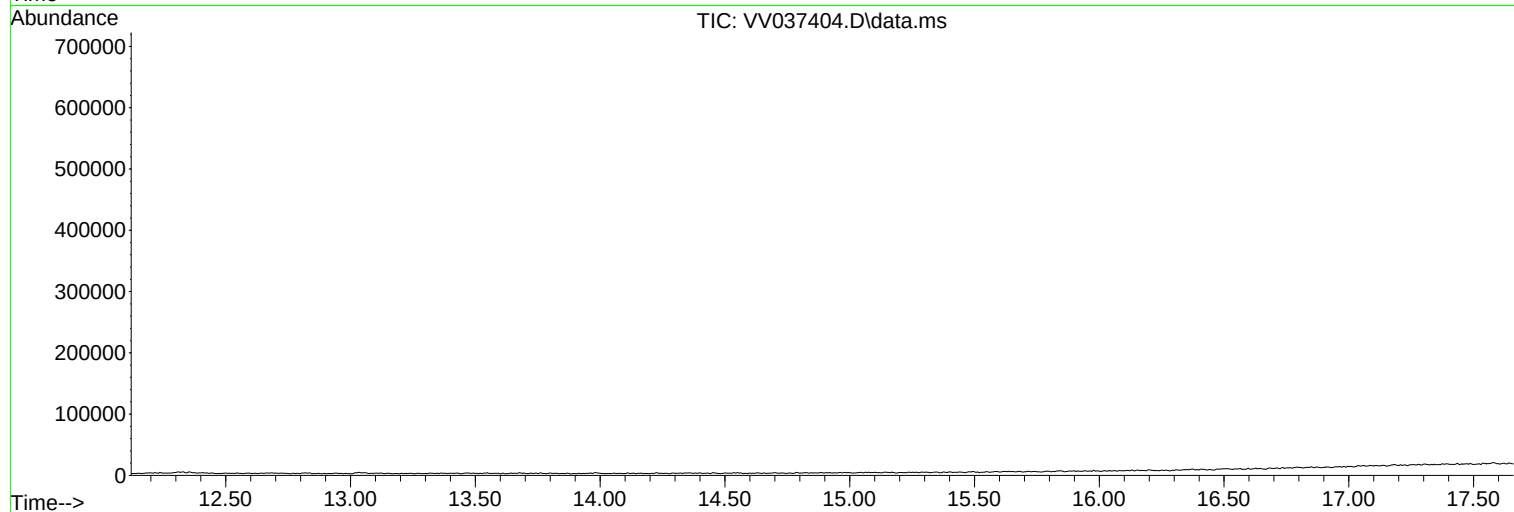
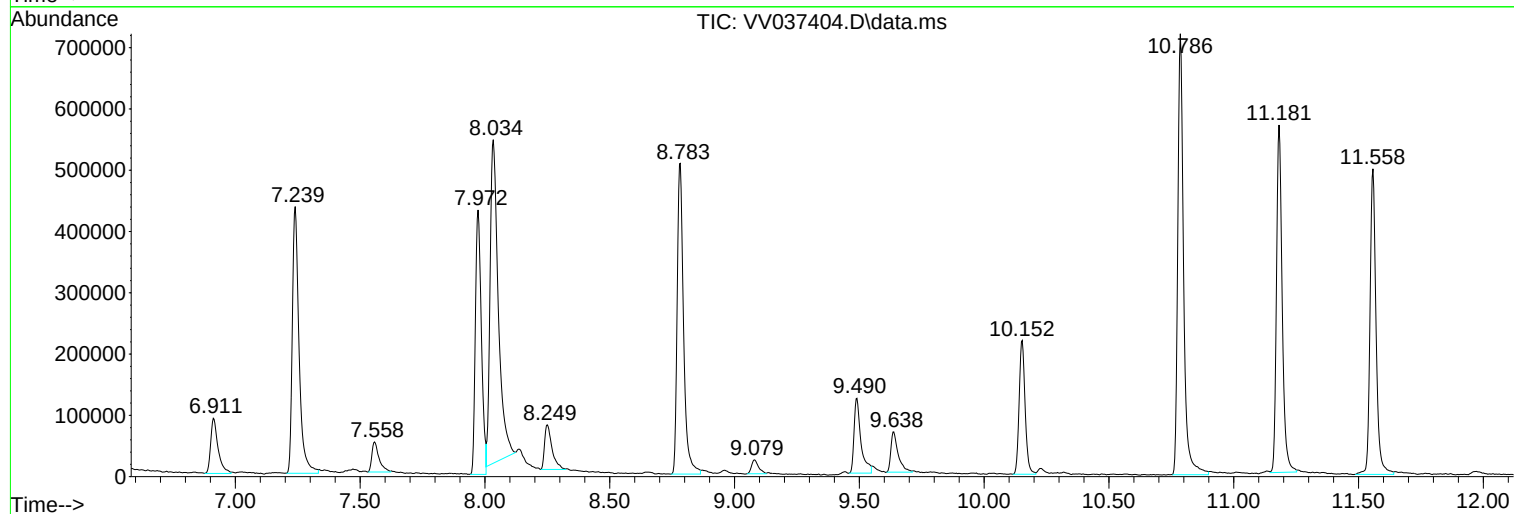
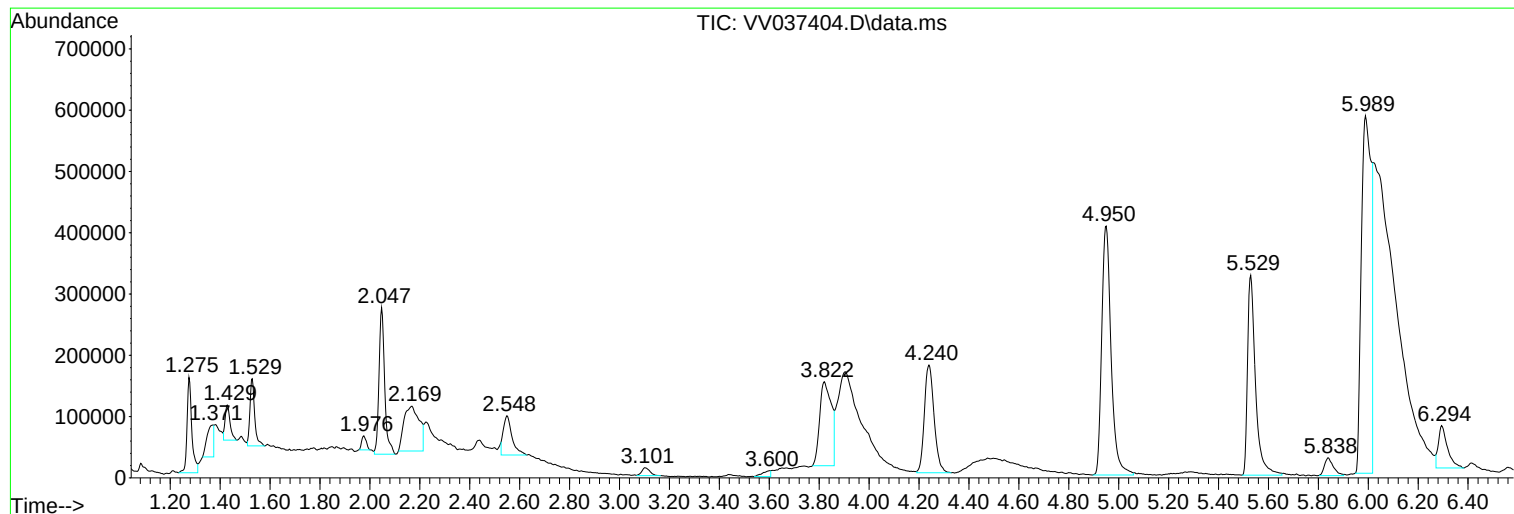
Sum of corrected areas: 13823331

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV091924\
Data File : VV037404.D
Acq On : 20 Sep 2024 00:42
Operator : SY/MD
Sample : P3988-14 20X
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8S3

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV091924\
Data File : VV037404.D
Acq On : 20 Sep 2024 00:42
Operator : SY/MD
Sample : P3988-14 20X
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8S3

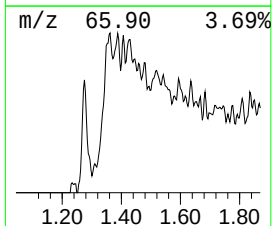
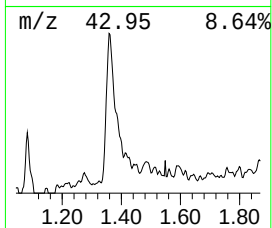
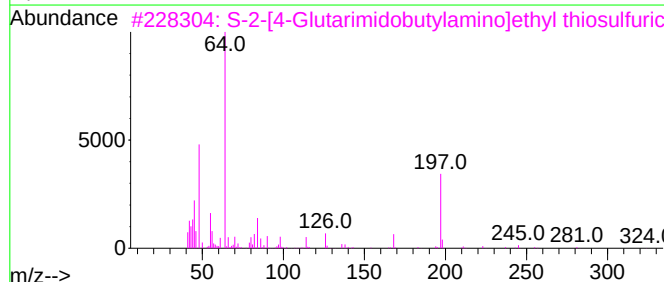
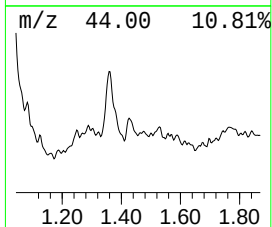
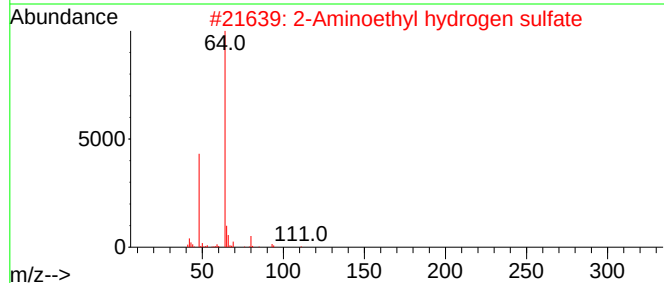
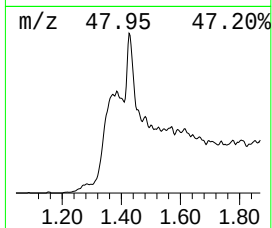
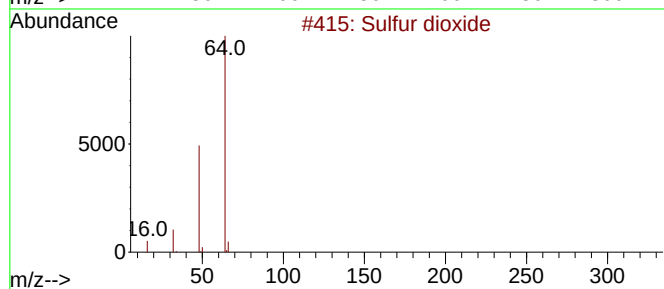
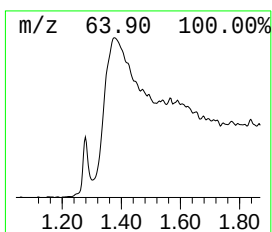
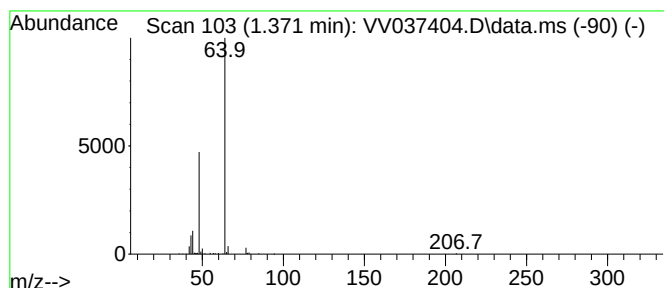
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR091024WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Sulfur dioxide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.371	0.68 ug/L	98388	1,4-Difluorobenzene	5.529

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	86
2			2-Aminoethyl hydrogen sulfate	141	C2H7N04S	000926-39-6	74
3			S-2-[4-Glutarimidobutylamino]eth...	324	C11H20N2O5S2	031701-78-7	64
4			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	64
5			Aminomethanesulfonic acid	111	CH5N03S	013881-91-9	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV091924\
Data File : VV037404.D
Acq On : 20 Sep 2024 00:42
Operator : SY/MD
Sample : P3988-14 20X
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8S3

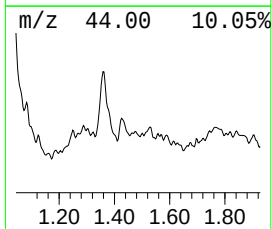
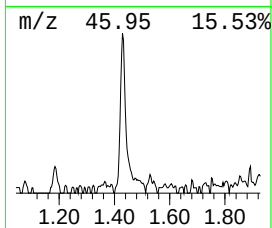
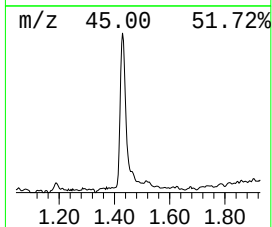
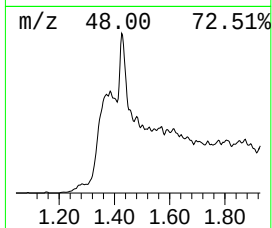
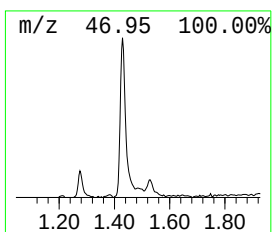
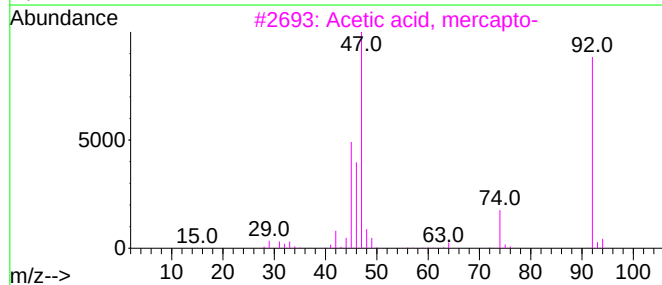
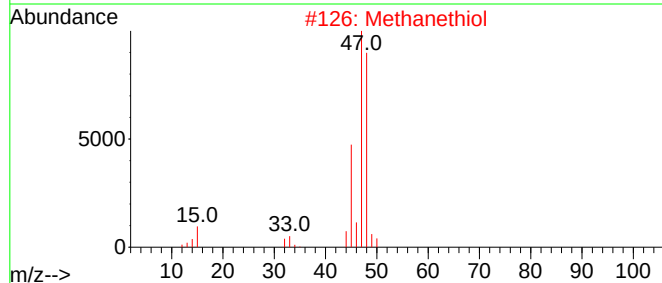
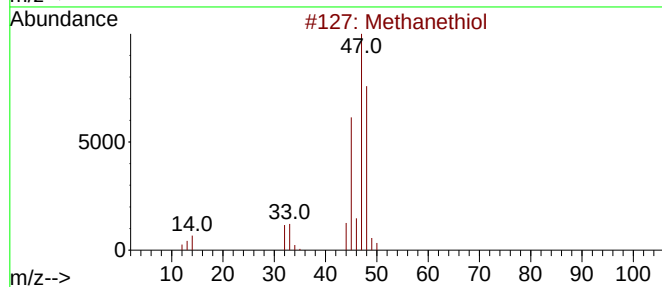
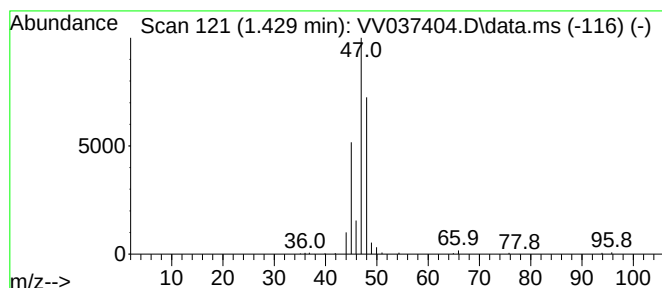
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR091024WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Methanethiol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.429	0.54 ug/L	78371	1,4-Difluorobenzene	5.529

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	9
4			Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	9
5			Acetic acid, mercapto-	92	C2H4O2S	000068-11-1	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV091924\
Data File : VV037404.D
Acq On : 20 Sep 2024 00:42
Operator : SY/MD
Sample : P3988-14 20X
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8S3

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

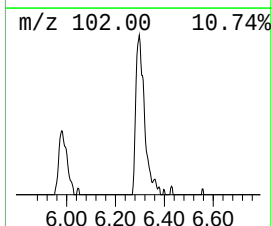
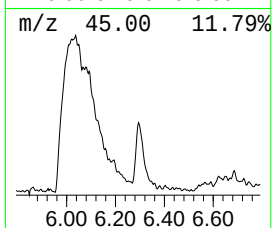
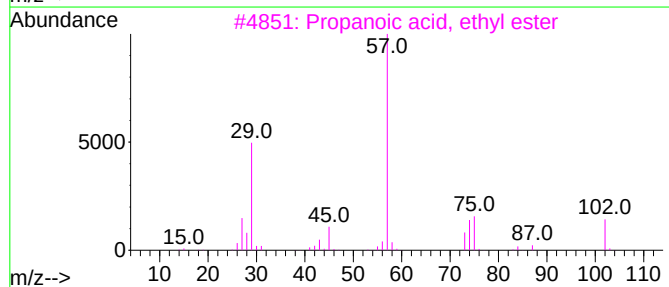
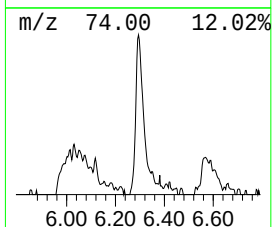
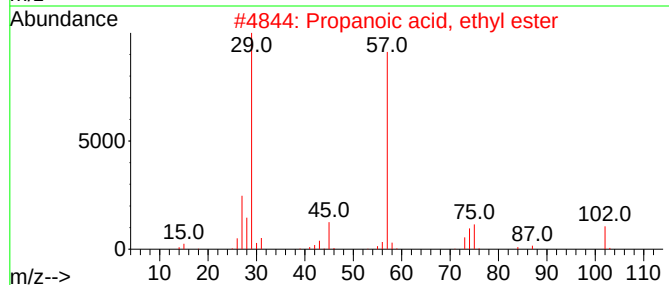
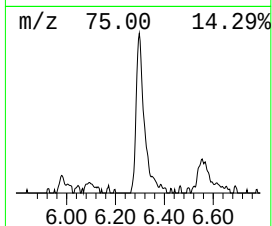
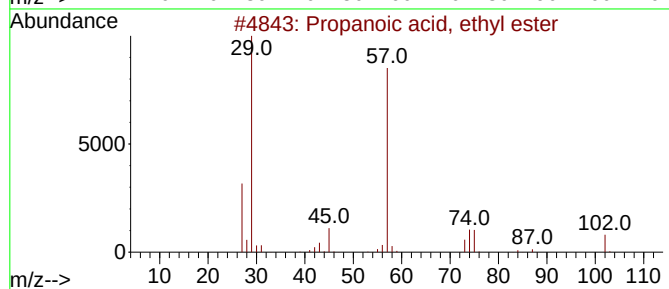
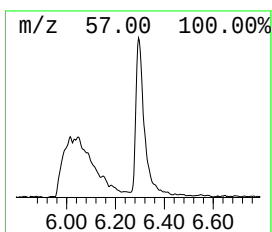
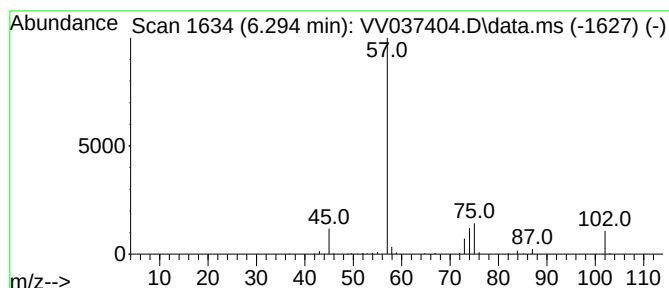
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 Propanoic acid, ethyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.294	1.19 ug/L	172923	1,4-Difluorobenzene	5.529

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, ethyl ester	102	C5H10O2	000105-37-3	86		
2	Propanoic acid, ethyl ester	102	C5H10O2	000105-37-3	86		
3	Propanoic acid, ethyl ester	102	C5H10O2	000105-37-3	72		
4	Propanoic acid, ethyl ester	102	C5H10O2	000105-37-3	64		
5	Propanoic acid, ethyl ester	102	C5H10O2	000105-37-3	53		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV091924\
Data File : VV037404.D
Acq On : 20 Sep 2024 00:42
Operator : SY/MD
Sample : P3988-14 20X
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8S3

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

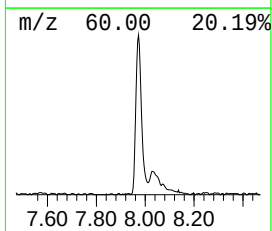
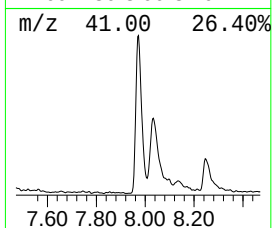
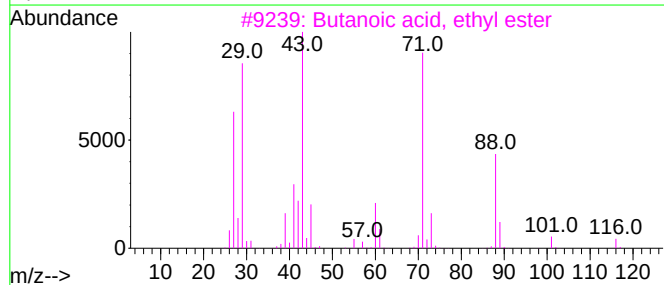
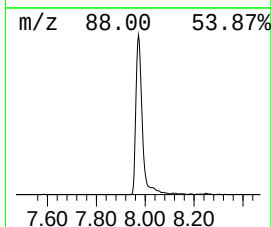
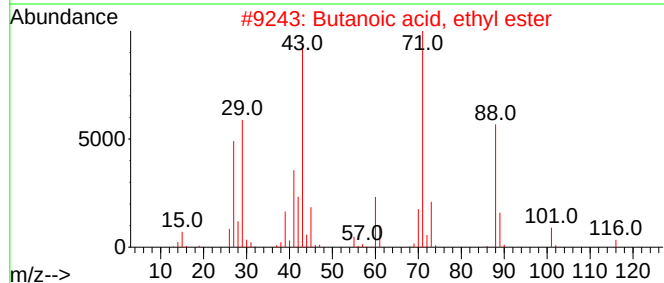
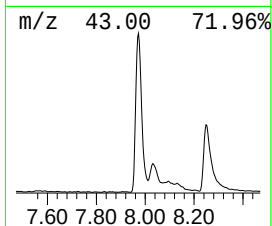
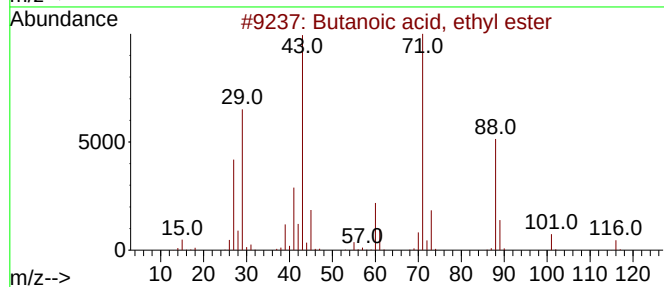
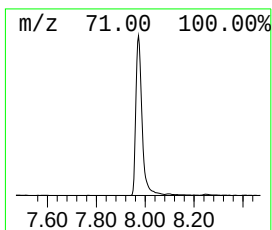
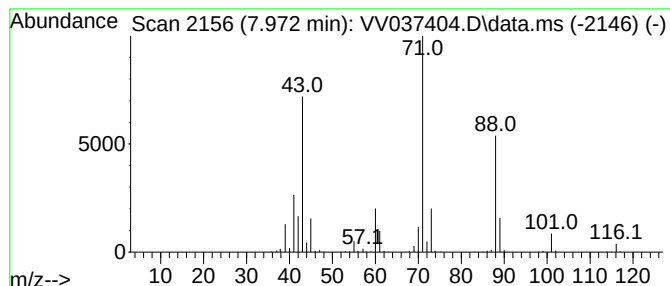
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 6 Butanoic acid, ethyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.972	3.99 ug/L	719815	Chlorobenzene-d5	8.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	94
2			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	94
3			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	90
4			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	90
5			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	83



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV091924\
Data File : VV037404.D
Acq On : 20 Sep 2024 00:42
Operator : SY/MD
Sample : P3988-14 20X
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8S3

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

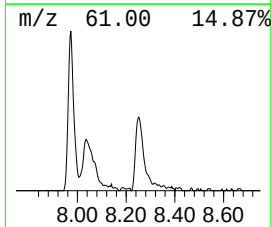
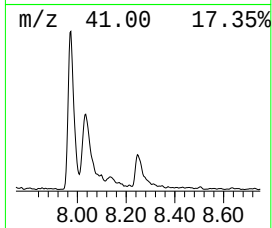
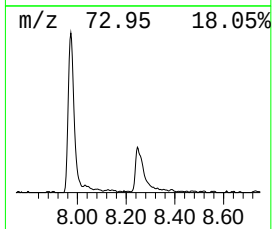
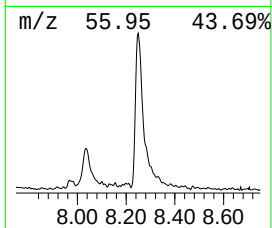
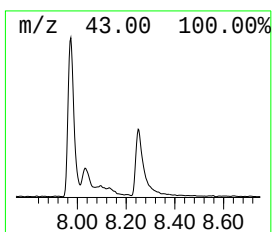
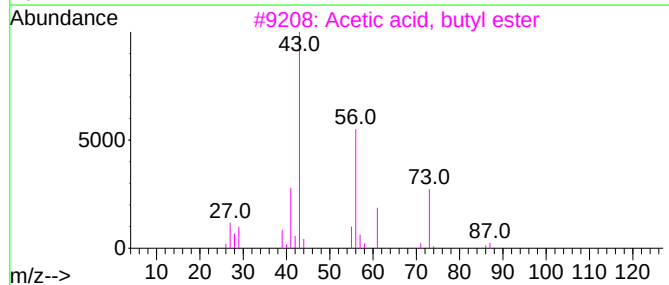
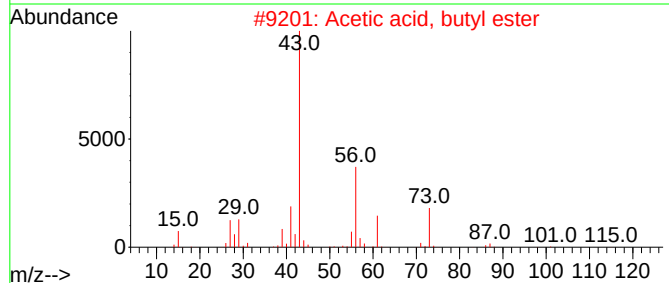
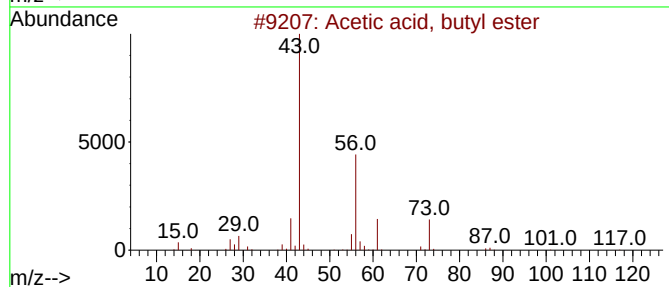
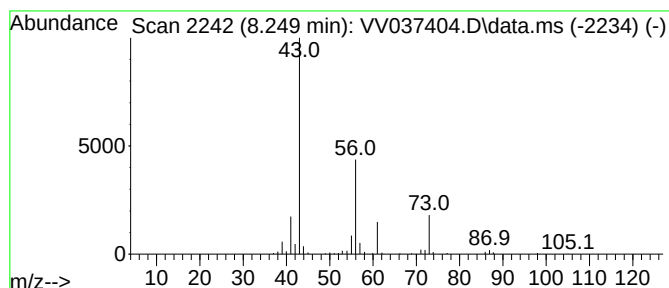
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 7 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.249	0.84 ug/L	151464	Chlorobenzene-d5	8.783

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	78
3	Acetic acid, butyl ester			116	C6H12O2	000123-86-4	50
4	Isobutyl acetate			116	C6H12O2	000110-19-0	40
5	Isobutyl acetate			116	C6H12O2	000110-19-0	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV091924\
Data File : VV037404.D
Acq On : 20 Sep 2024 00:42
Operator : SY/MD
Sample : P3988-14 20X
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8S3

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

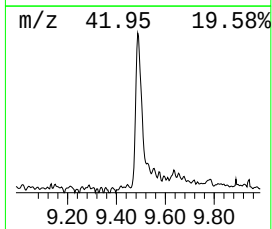
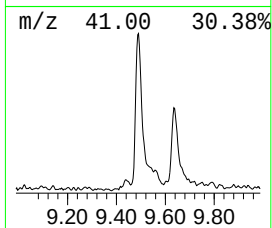
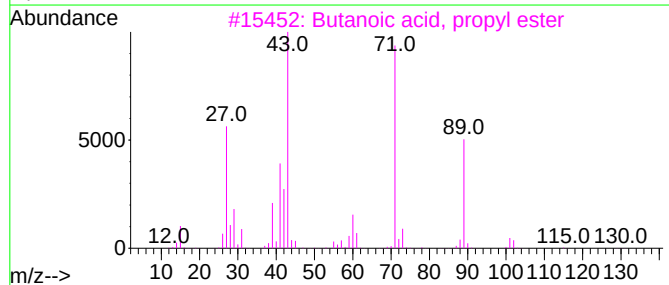
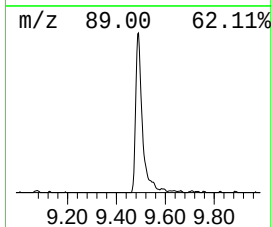
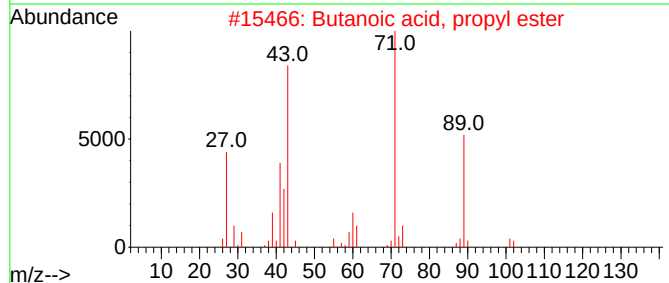
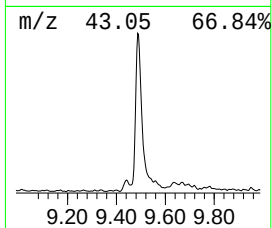
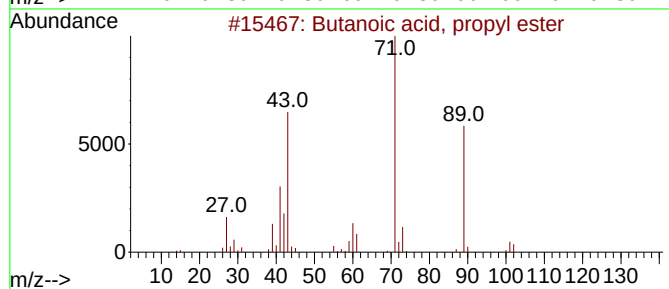
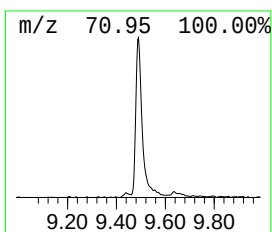
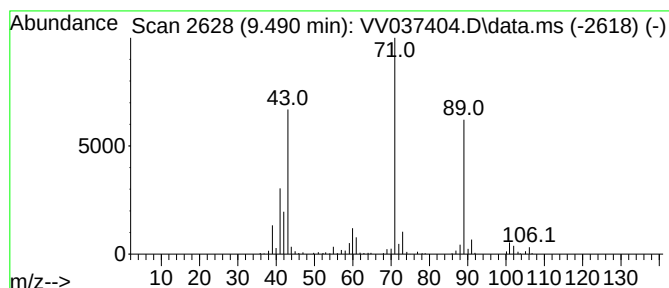
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 8 Butanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.490	1.31 ug/L	235537	Chlorobenzene-d5	8.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
2			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	86
3			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	83
4			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	72
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV091924\
Data File : VV037404.D
Acq On : 20 Sep 2024 00:42
Operator : SY/MD
Sample : P3988-14 20X
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8S3

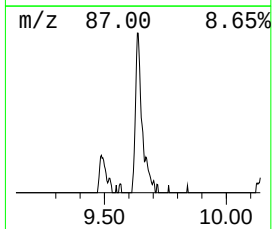
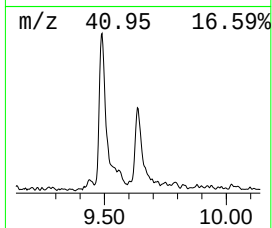
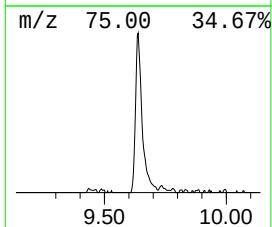
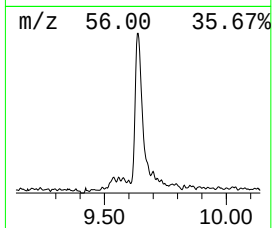
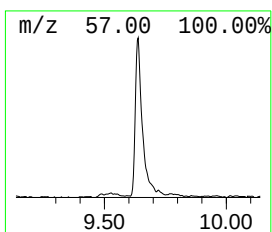
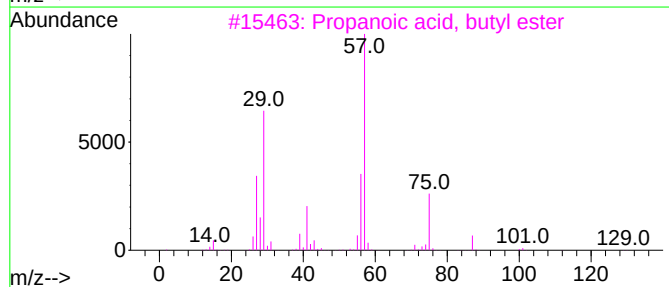
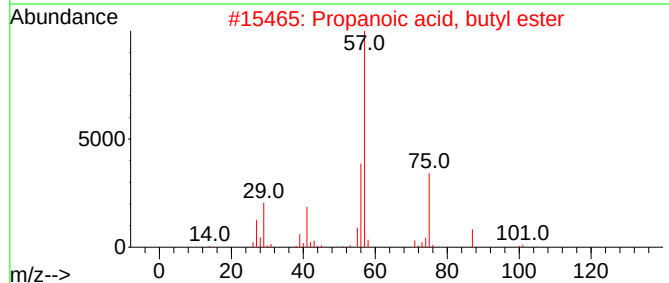
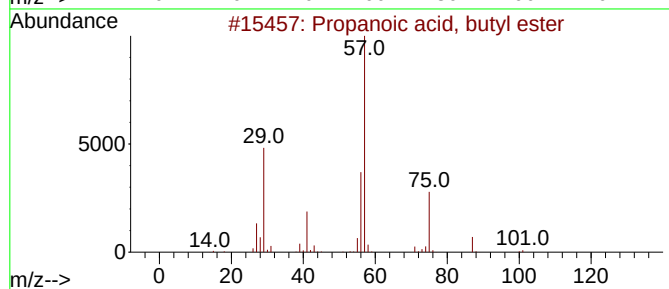
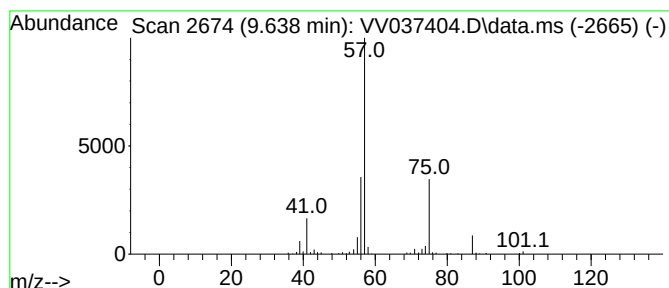
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR091024WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 Propanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.638	0.74 ug/L	133523	Chlorobenzene-d5	8.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, butyl ester		130	C7H14O2	000590-01-2	83	
2	Propanoic acid, butyl ester		130	C7H14O2	000590-01-2	83	
3	Propanoic acid, butyl ester		130	C7H14O2	000590-01-2	72	
4	Propanoic acid, butyl ester		130	C7H14O2	000590-01-2	64	
5	Propanoic acid, 2-methylpropyl e...		130	C7H14O2	000540-42-1	33	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV091924\
Data File : VV037404.D
Acq On : 20 Sep 2024 00:42
Operator : SY/MD
Sample : P3988-14 20X
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8S3

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

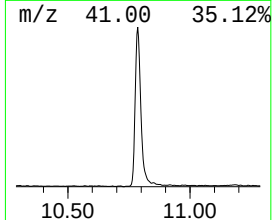
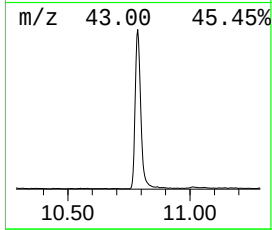
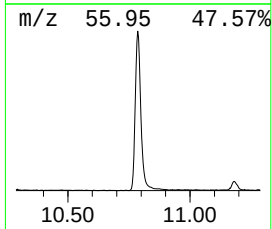
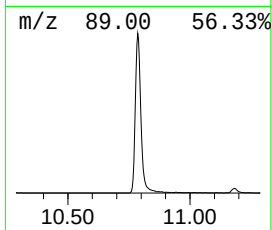
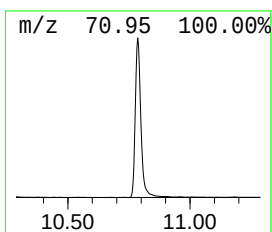
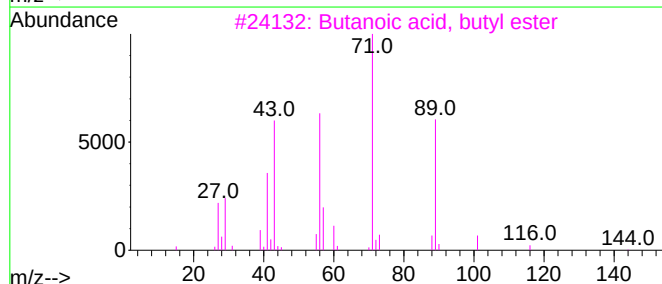
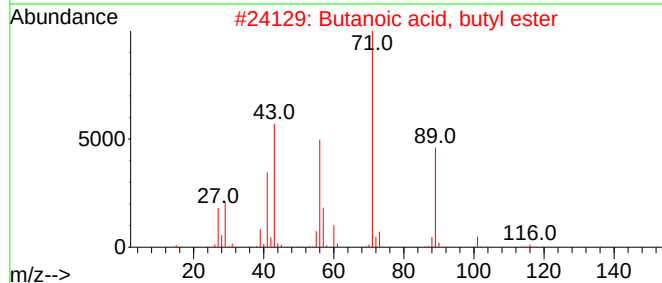
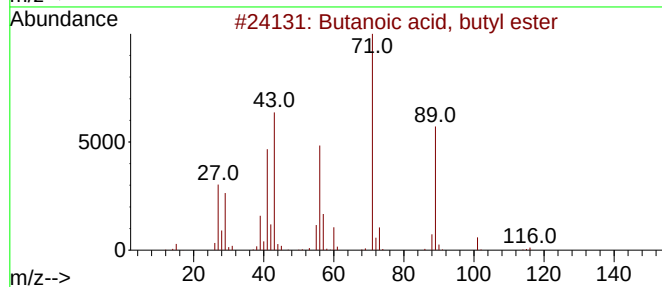
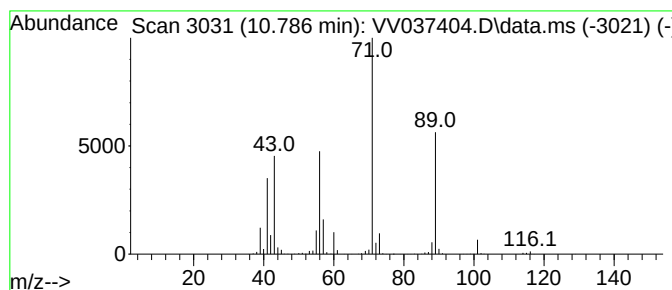
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 10 Butanoic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.786	6.47 ug/L	1169860	1,4-Dichlorobenzene-d4	11.181

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	86
3			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	83
4			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	72
5			Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV091924\
Data File : VV037404.D
Acq On : 20 Sep 2024 00:42
Operator : SY/MD
Sample : P3988-14 20X
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
BH8S3

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
Sulfur dioxide	1.371	0.7	ug/L	98388	1	5.529	726720	5.0
Methanethiol	1.429	0.5	ug/L	78371	1	5.529	726720	5.0
Propanoic acid,...	6.294	1.2	ug/L	172923	1	5.529	726720	5.0
Butanoic acid, ...	7.972	4.0	ug/L	719815	2	8.783	901566	5.0
Acetic acid, bu...	8.249	0.8	ug/L	151464	2	8.783	901566	5.0
Butanoic acid, ...	9.490	1.3	ug/L	235537	2	8.783	901566	5.0
Propanoic acid,...	9.638	0.7	ug/L	133523	2	8.783	901566	5.0
Butanoic acid, ...	10.786	6.5	ug/L	1169860	3	11.181	903999	5.0