

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
 Data File : VX033855.D
 Acq On : 23 Jan 2023 17:29
 Operator : JC/MD
 Sample : 01251-08
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMP-2

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

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_X\Method\82X011123W.M
 Title : SW846 8260

Signal : TIC: VX033855.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.392	207	214	224	rBV	10633	21858	1.43%	0.236%
2	2.788	273	279	291	rBV	15821	31062	2.03%	0.335%
3	4.715	586	595	615	rBV	10818	33145	2.17%	0.358%
4	5.385	693	705	721	rBV2	79086	235490	15.41%	2.542%
5	5.550	721	732	747	rVB	143521	410911	26.89%	4.436%
6	5.952	785	798	816	rBV	79991	217770	14.25%	2.351%
7	6.342	851	862	878	rBV	61942	162937	10.66%	1.759%
8	6.763	921	931	942	rBV	214343	536653	35.11%	5.793%
9	7.641	1065	1075	1080	rBV	33878	65068	4.26%	0.702%
10	7.690	1080	1083	1093	rVB	11668	21772	1.42%	0.235%
11	7.799	1093	1101	1120	rBV	857845	1528332	100.00%	16.499%
12	8.549	1217	1224	1234	rBV	185209	299435	19.59%	3.233%
13	8.647	1234	1240	1256	rVB	444959	699084	45.74%	7.547%
14	8.952	1284	1290	1302	rBV	261182	374134	24.48%	4.039%
15	9.244	1332	1338	1344	rBV	265797	371396	24.30%	4.009%
16	9.305	1344	1348	1351	rVV	23032	35891	2.35%	0.387%
17	9.342	1351	1354	1356	rVV	41291	55388	3.62%	0.598%
18	9.378	1356	1360	1368	rVV	103256	155885	10.20%	1.683%
19	9.482	1372	1377	1388	rVV	462313	611966	40.04%	6.606%
20	9.580	1388	1393	1404	rVB	307781	405380	26.52%	4.376%
21	9.915	1442	1448	1463	rBV	817643	1092482	71.48%	11.794%
22	10.055	1463	1471	1478	rBV	427399	593552	38.84%	6.408%
23	10.281	1503	1508	1515	rBV	10731	16689	1.09%	0.180%
24	10.506	1540	1545	1551	rBV	11590	15618	1.02%	0.169%
25	10.640	1562	1567	1579	rBV	77785	101512	6.64%	1.096%
26	11.079	1634	1639	1650	rBV	352180	442877	28.98%	4.781%
27	12.024	1788	1794	1801	rBV	398200	514027	33.63%	5.549%
28	13.774	2076	2081	2089	rBV	116185	141703	9.27%	1.530%
29	14.640	2219	2223	2233	rVB	25254	33266	2.18%	0.359%
30	14.780	2241	2246	2254	rBV	30476	37911	2.48%	0.409%

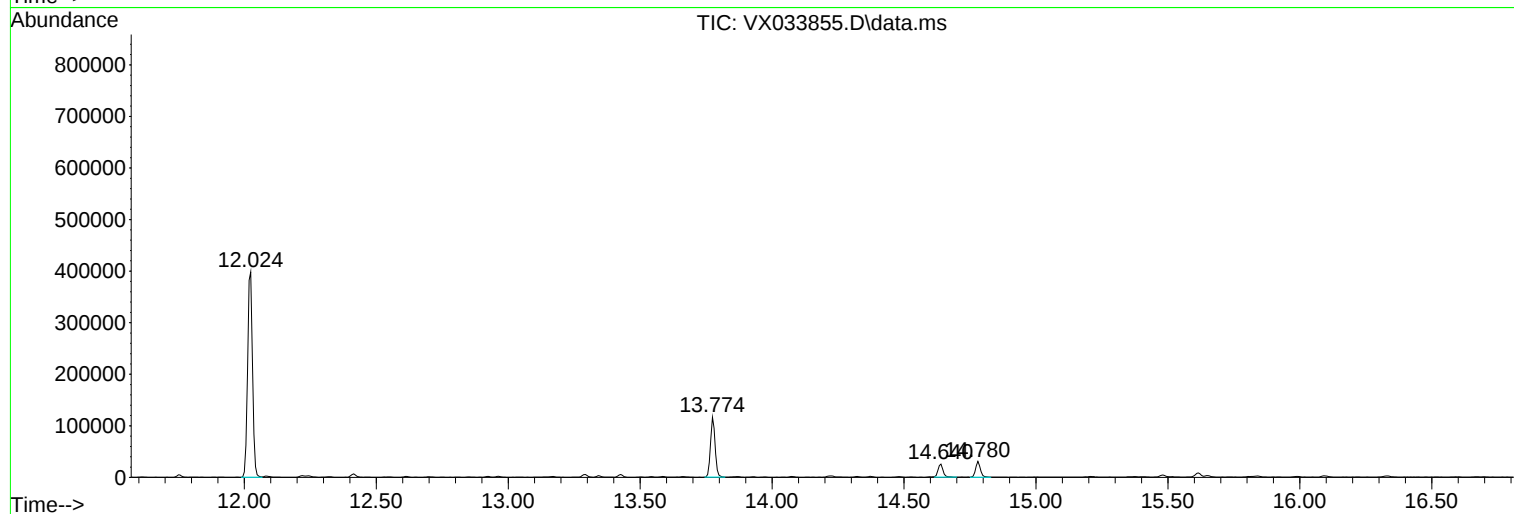
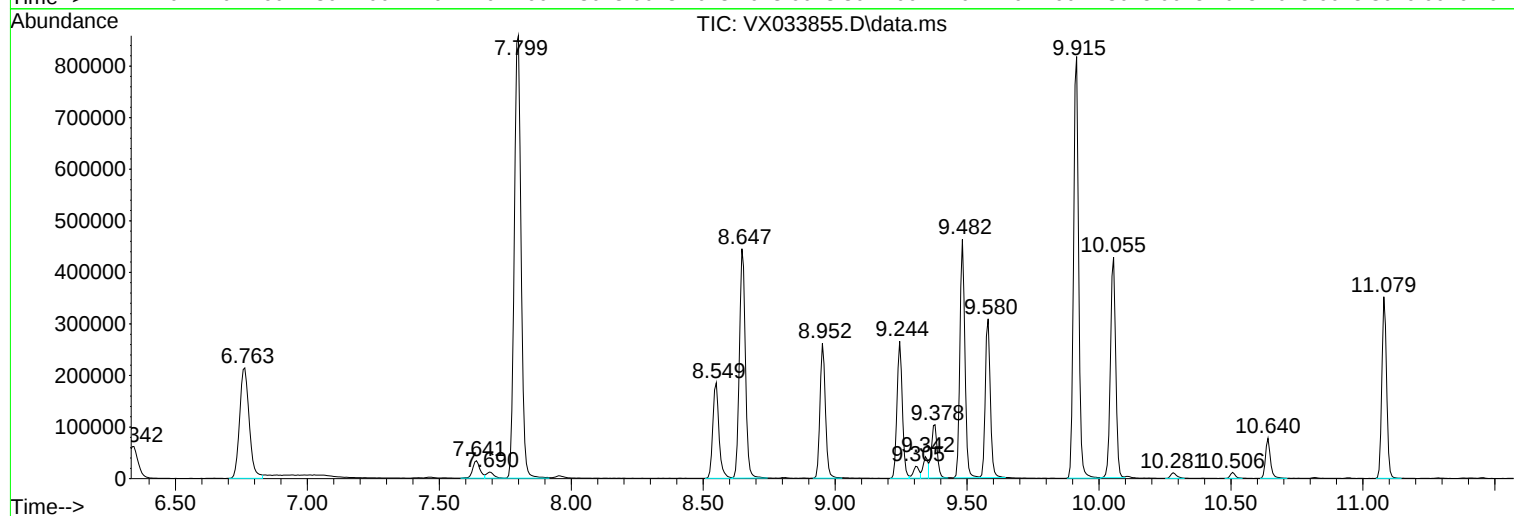
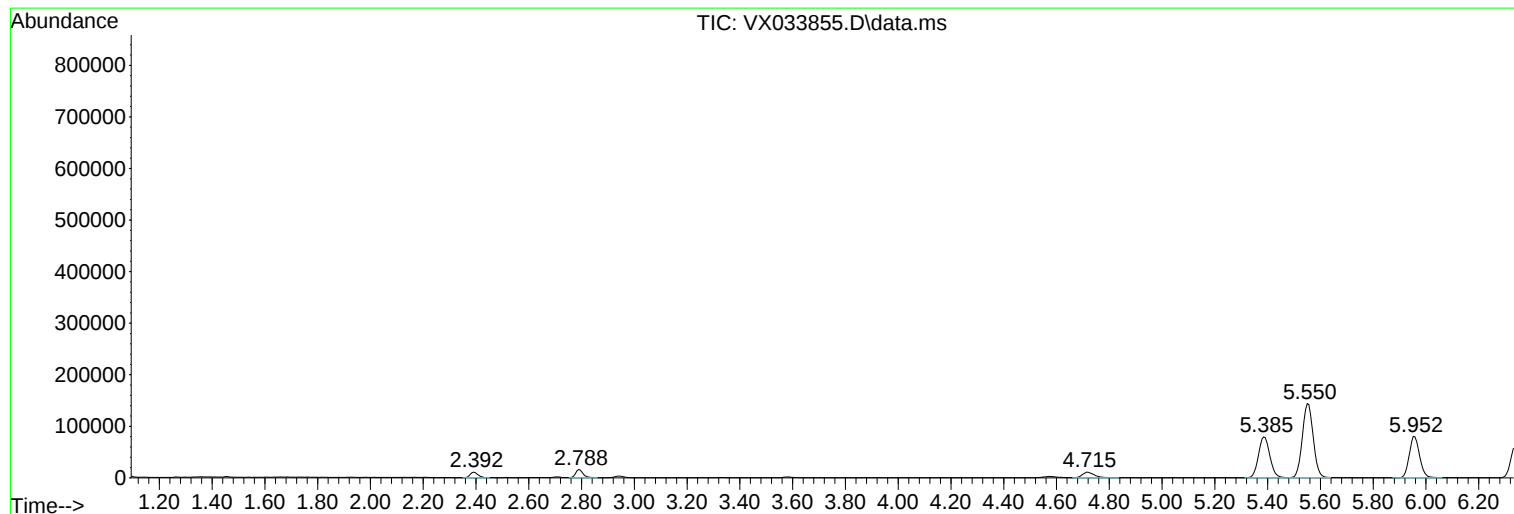
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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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



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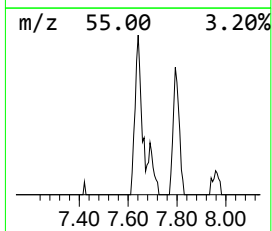
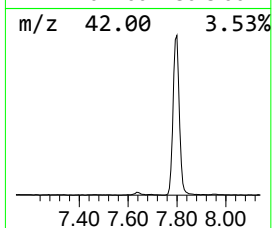
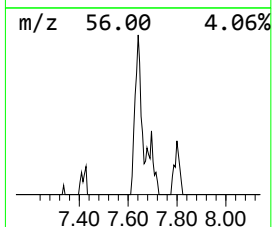
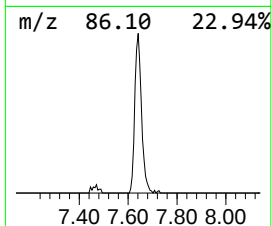
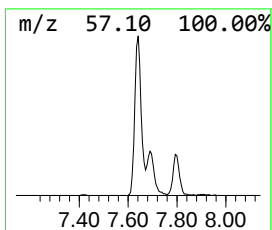
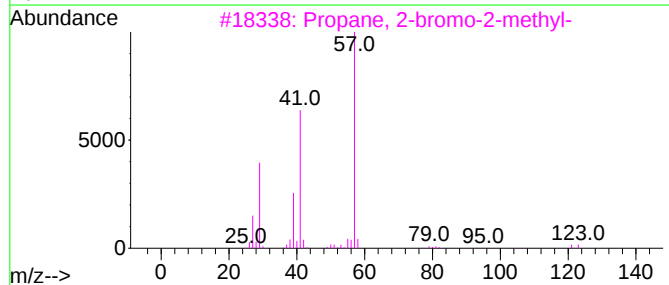
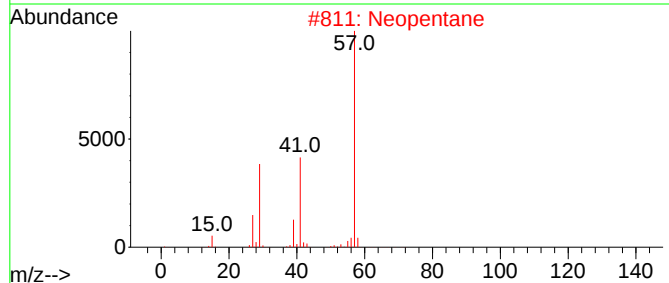
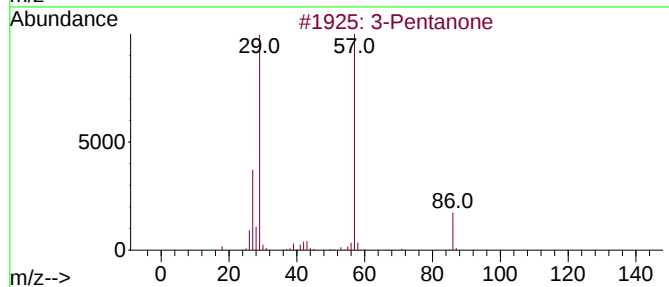
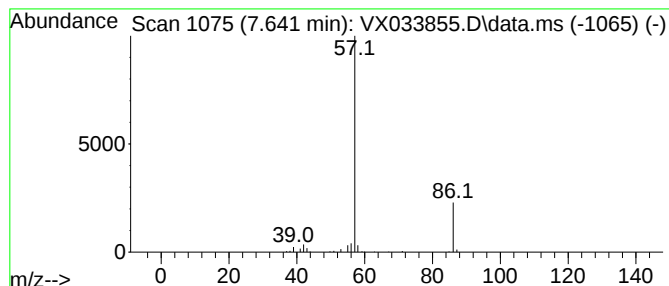
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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

Peak Number 1 3-Pentanone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.641	6.06 ug/l	65068	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone	86	C5H10O	000096-22-0	86
2			Neopentane	72	C5H12	000463-82-1	9
3			Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	9
4			Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	9
5			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	7



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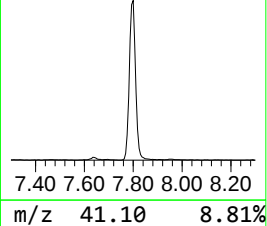
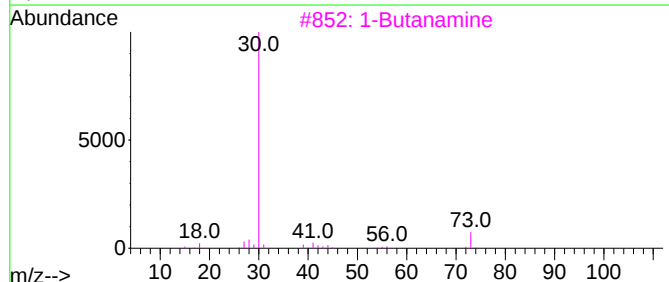
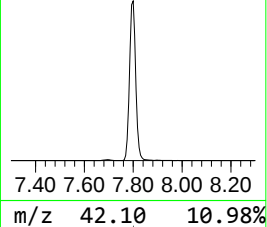
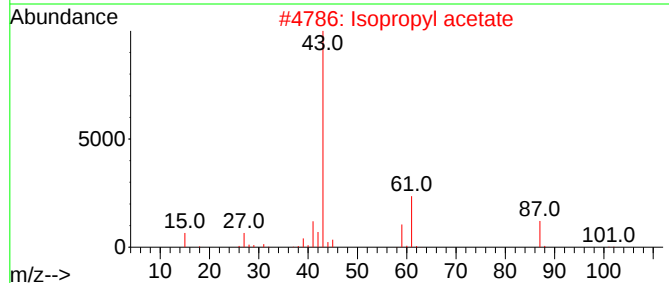
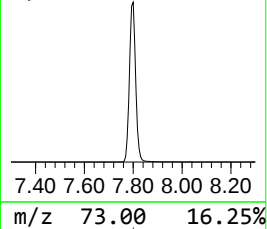
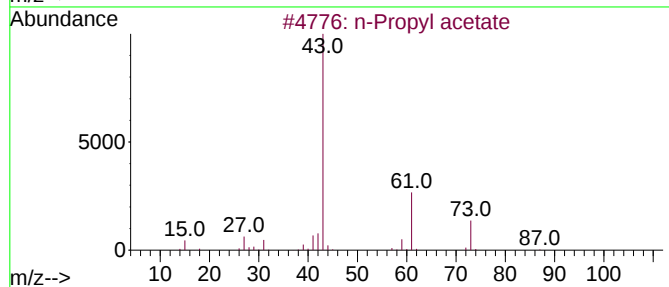
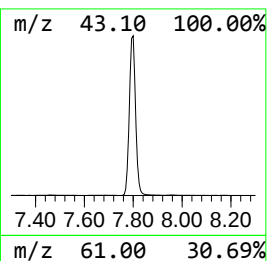
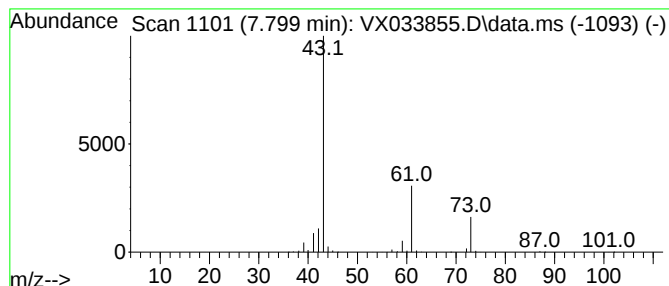
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	142.40 ug/l	1528330	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Propyl acetate	102	C5H10O2	000109-60-4	83
2			Isopropyl acetate	102	C5H10O2	000108-21-4	36
3			1-Butanamine	73	C4H11N	000109-73-9	7
4			Isobutylamine	73	C4H11N	000078-81-9	4
5			N-Acetythylenediamine	102	C4H10N2O	001001-53-2	4



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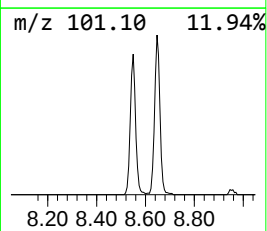
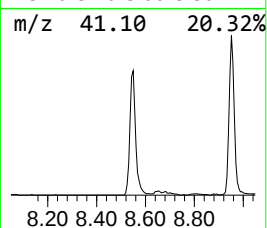
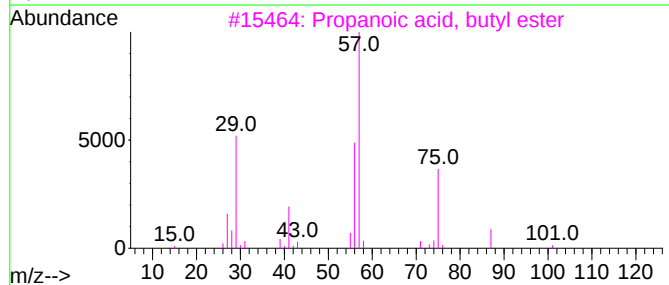
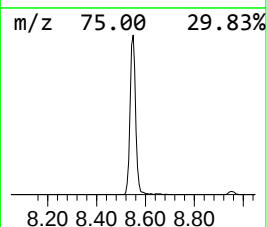
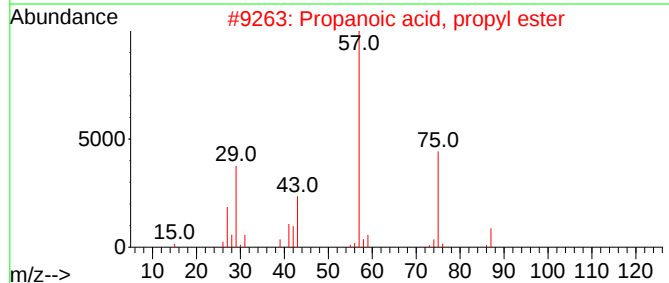
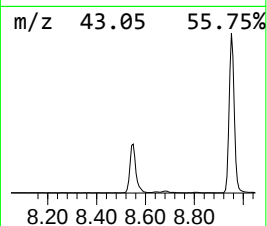
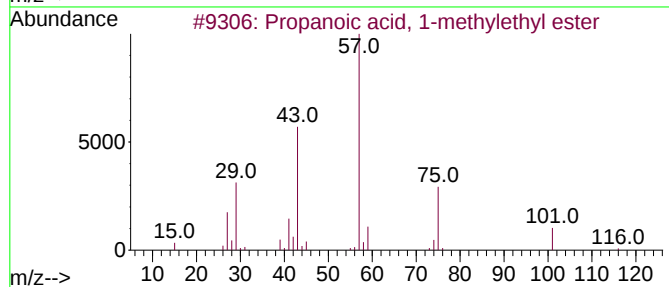
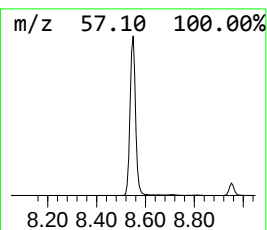
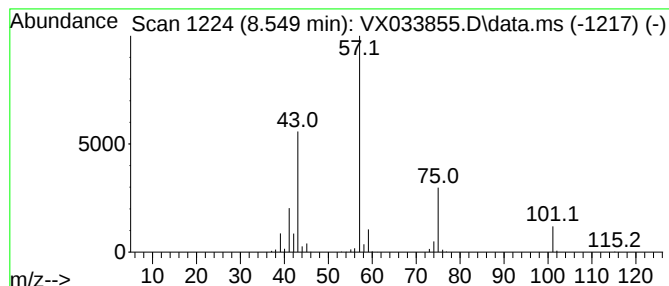
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.549	25.22 ug/l	299435	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
2			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
3			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
4			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	10
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10



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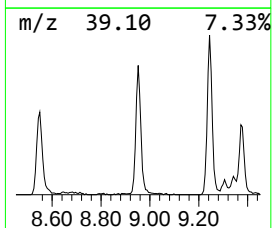
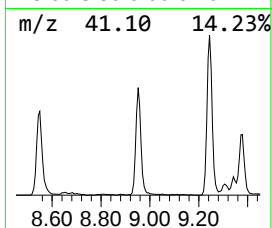
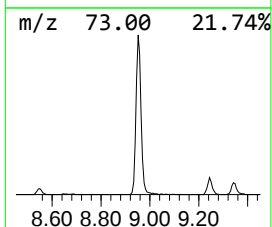
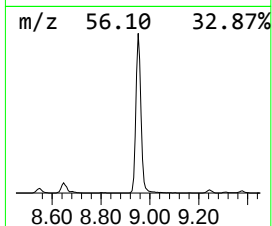
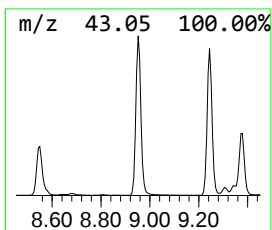
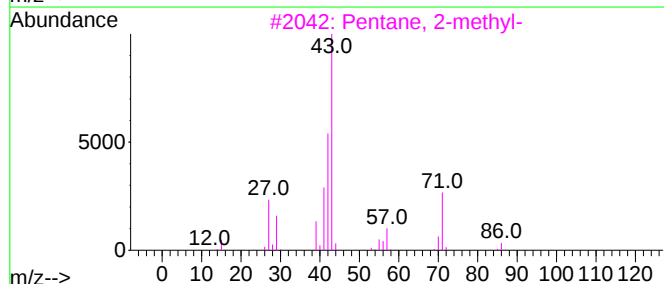
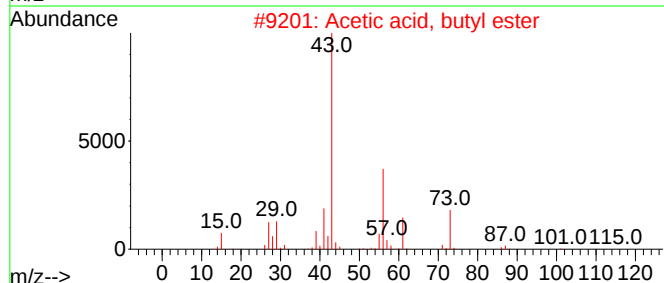
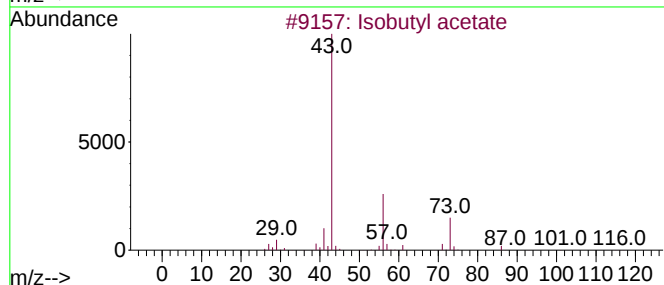
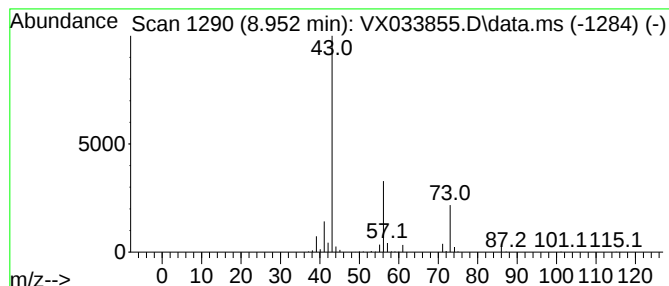
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Isobutyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.952	31.52 ug/l	374134	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutyl acetate	116	C6H12O2	000110-19-0	83
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	38
3			Pentane, 2-methyl-	86	C6H14	000107-83-5	9
4			Isobutylamine	73	C4H11N	000078-81-9	9
5			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9



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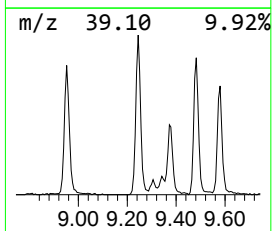
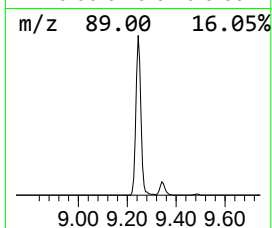
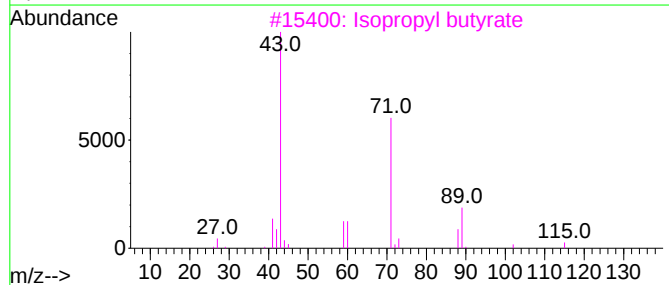
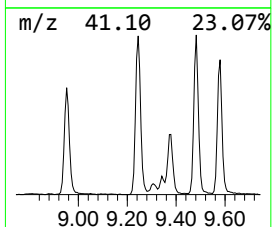
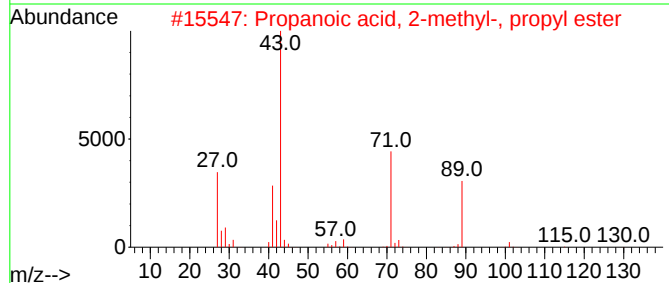
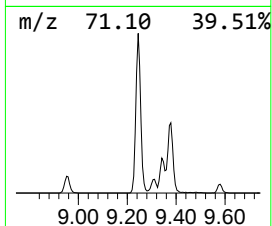
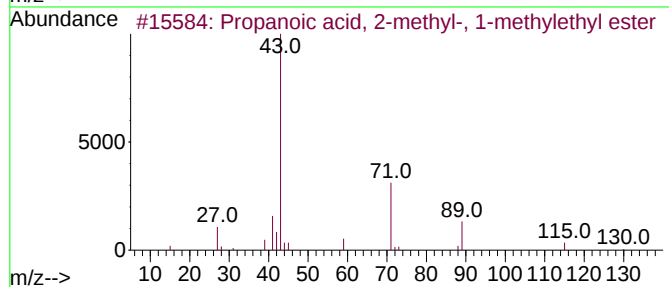
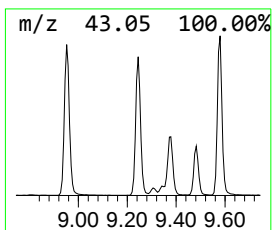
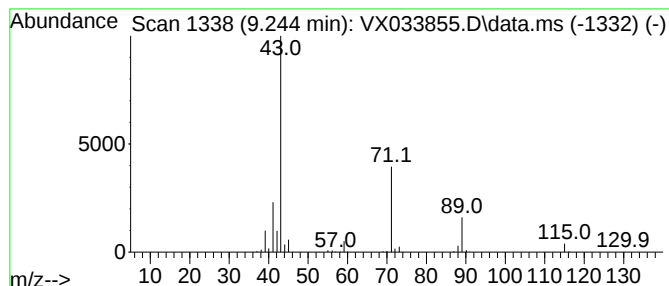
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.244	31.29 ug/l	371396	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	43
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	42
5			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42



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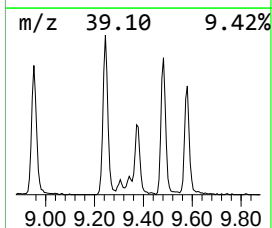
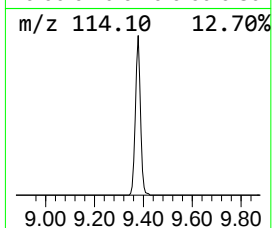
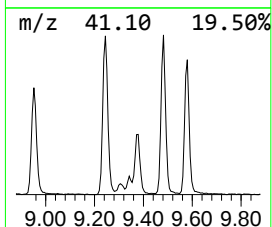
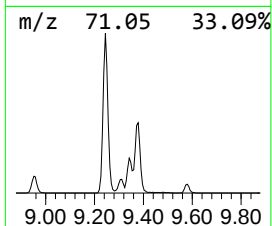
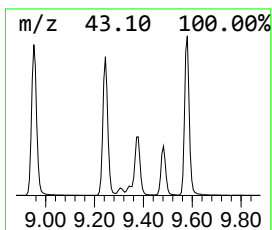
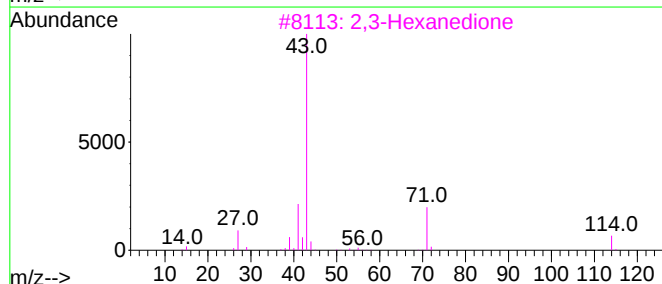
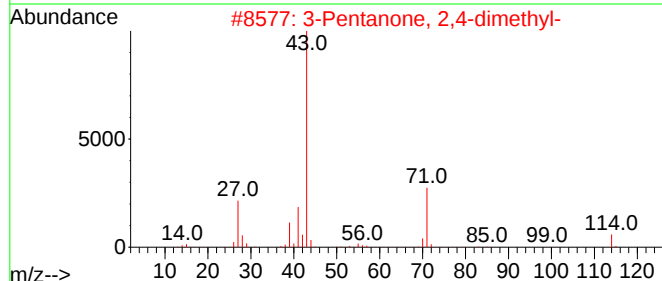
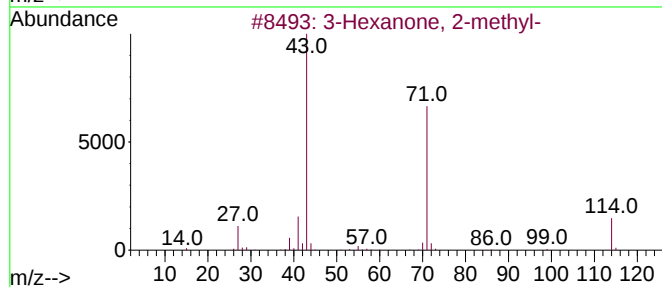
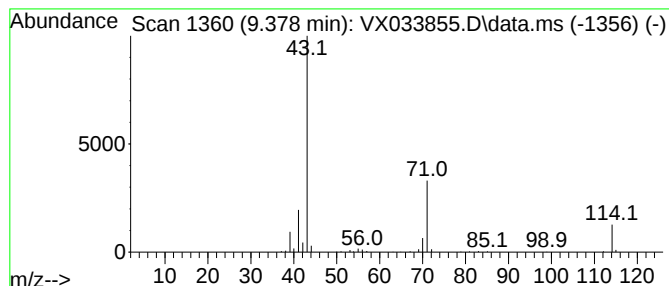
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Quant Title : SW846 8260

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

Peak Number 6 3-Hexanone, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.378	13.13 ug/l	155885	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	72
2			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	64
3			2,3-Hexanedione	114	C6H10O2	003848-24-6	64
4			Pyrrolidine	71	C4H9N	000123-75-1	47
5			3,4-Dimethyl-2-pentanone	114	C7H14O	1000202-23-1	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
Data File : VX033855.D
Acq On : 23 Jan 2023 17:29
Operator : JC/MD
Sample : 01251-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-2

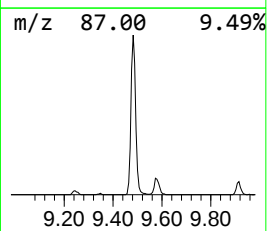
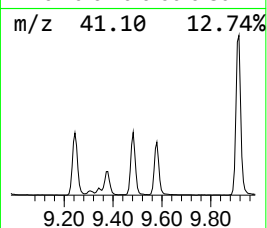
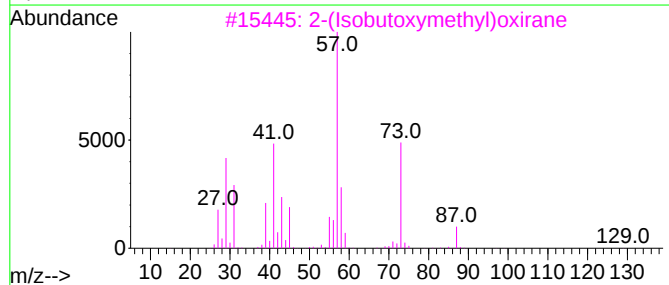
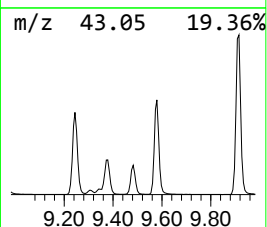
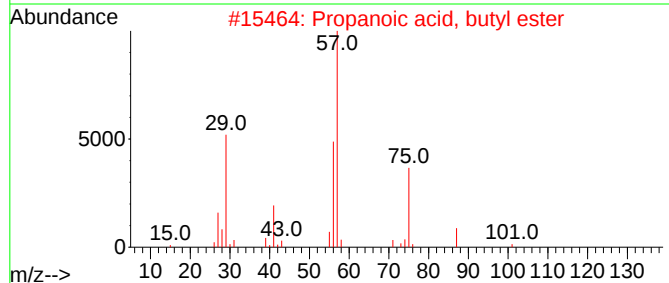
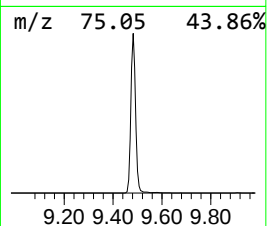
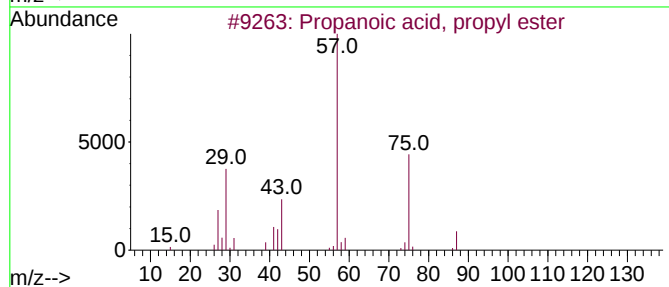
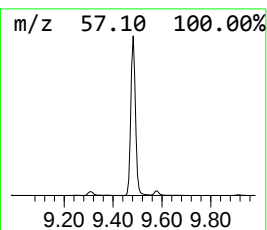
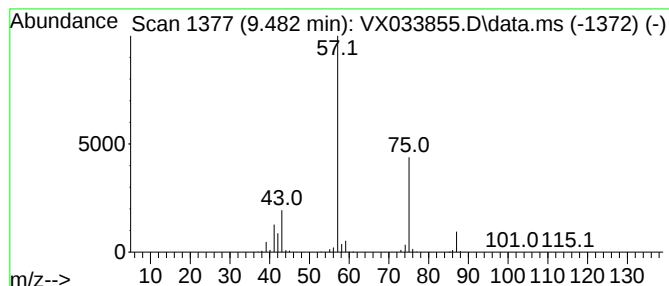
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Quant Title : SW846 8260

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

Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	51.55 ug/l	611966	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2			Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	40
3			2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
4			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
Data File : VX033855.D
Acq On : 23 Jan 2023 17:29
Operator : JC/MD
Sample : 01251-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-2

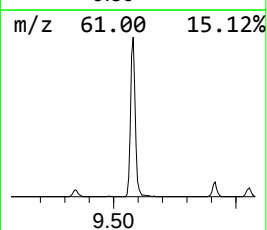
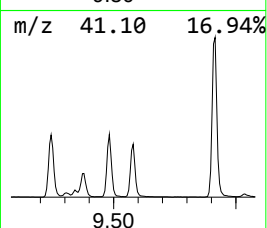
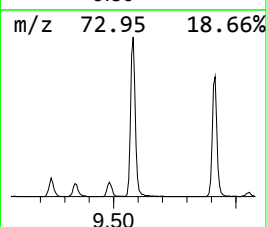
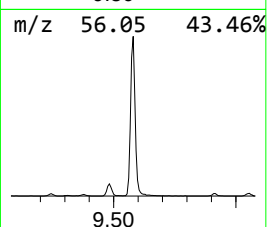
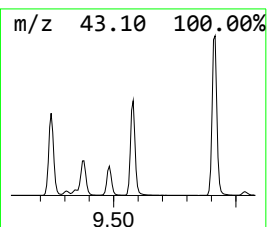
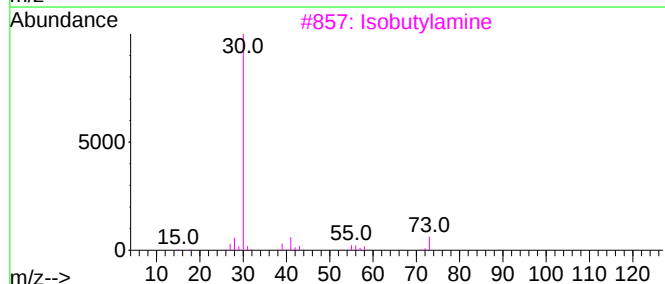
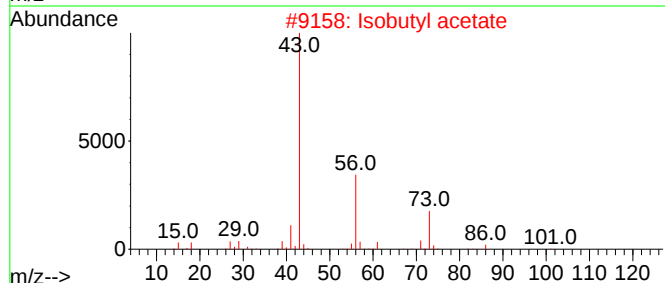
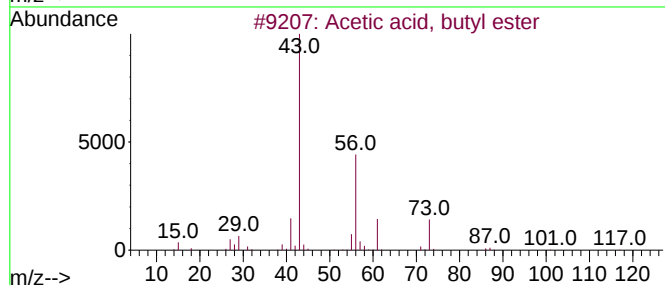
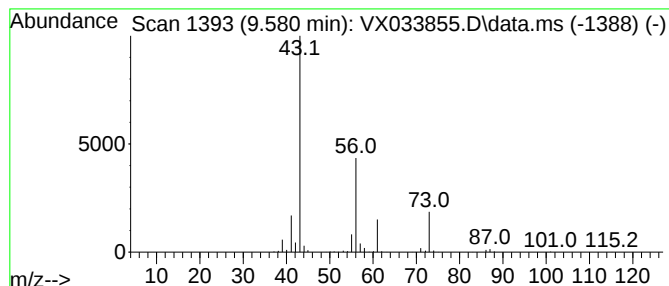
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Quant Title : SW846 8260

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

Peak Number 8 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	34.15 ug/l	405380	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	83
2			Isobutyl acetate	116	C6H12O2	000110-19-0	40
3			Isobutylamine	73	C4H11N	000078-81-9	9
4			Isopropyl acetate	102	C5H10O2	000108-21-4	9
5			Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
Data File : VX033855.D
Acq On : 23 Jan 2023 17:29
Operator : JC/MD
Sample : 01251-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-2

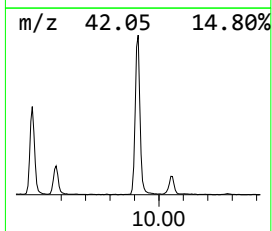
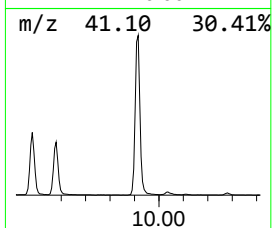
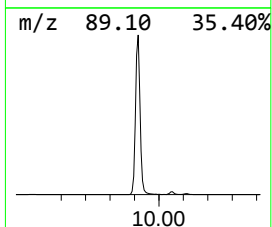
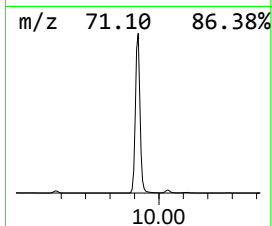
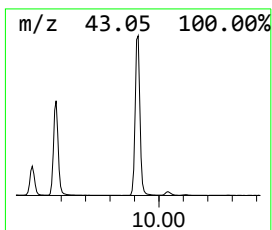
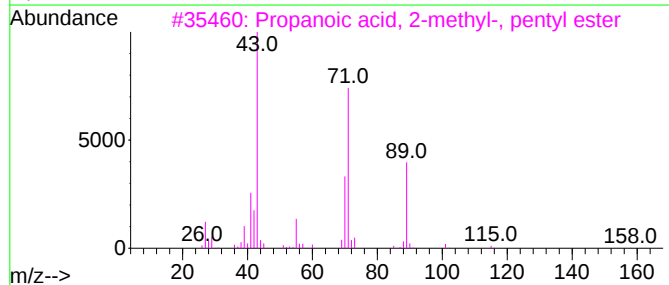
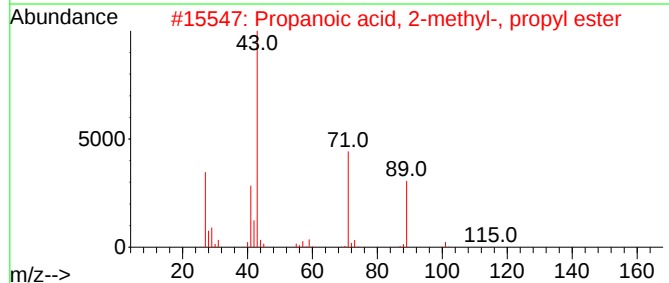
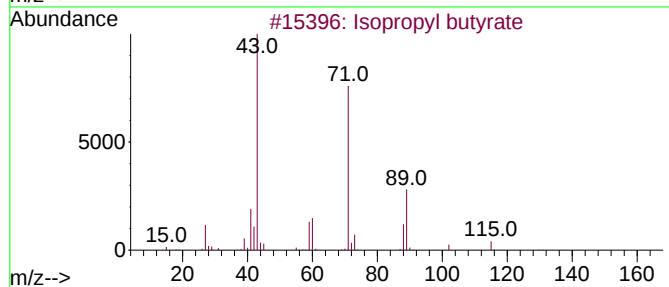
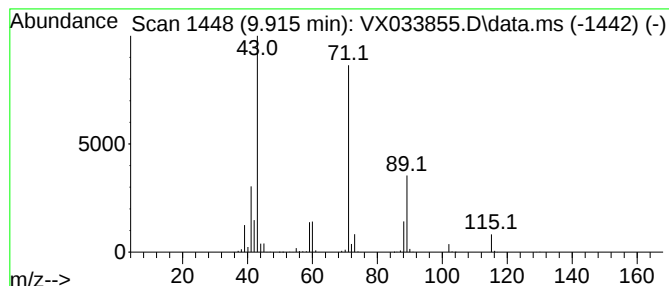
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Quant Title : SW846 8260

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

Peak Number 9 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	92.03 ug/l	1092480	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2			Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	72
3			Propanoic acid, 2-methyl-, pentyl...	158	C9H18O2	002445-72-9	64
4			Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
Data File : VX033855.D
Acq On : 23 Jan 2023 17:29
Operator : JC/MD
Sample : 01251-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-2

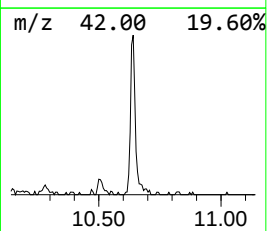
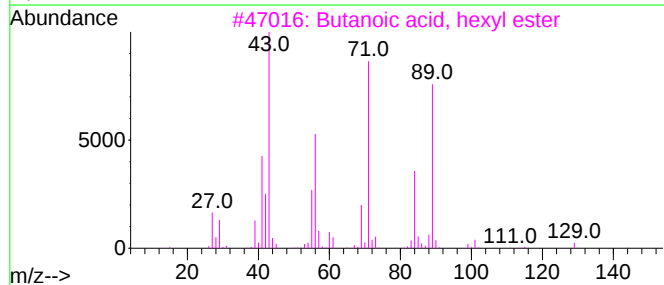
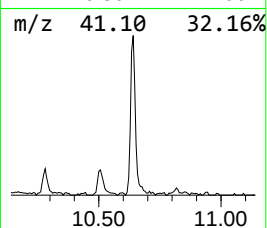
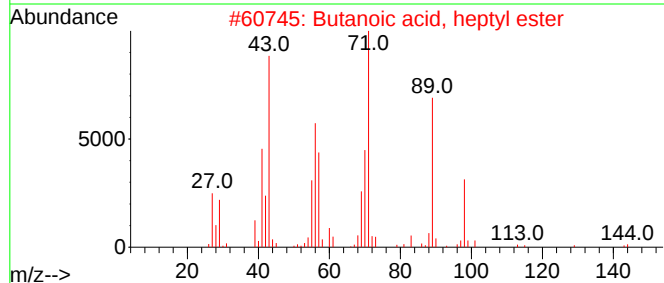
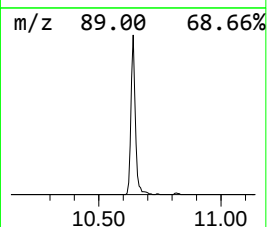
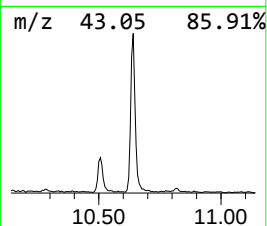
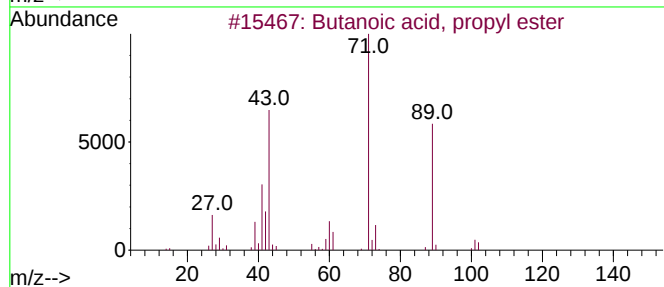
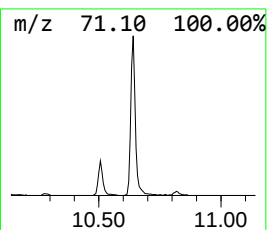
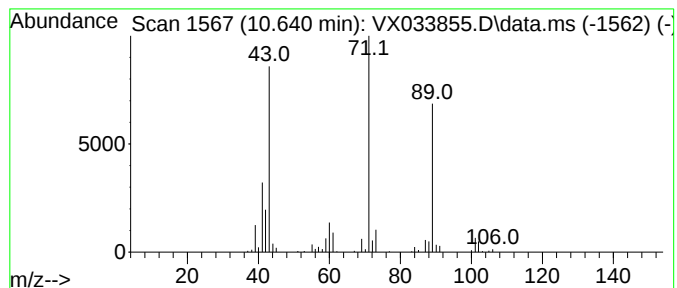
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

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

Peak Number 10 Butanoic acid, propyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.640	8.55 ug/l	101512	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	90
2			Butanoic acid, heptyl ester	186	C11H22O2	005870-93-9	78
3			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	78
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
5			Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX012323\
Data File : VX033855.D
Acq On : 23 Jan 2023 17:29
Operator : JC/MD
Sample : 01251-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011123W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Pentanone	7.641	6.1	ug/l	65068	2	6.763	536653	50.0
n-Propyl acetate	7.799	142.4	ug/l	1528330	2	6.763	536653	50.0
Propanoic acid,...	8.549	25.2	ug/l	299435	3	10.055	593552	50.0
Isobutyl acetate	8.952	31.5	ug/l	374134	3	10.055	593552	50.0
Propanoic acid,...	9.244	31.3	ug/l	371396	3	10.055	593552	50.0
3-Hexanone, 2-m...	9.378	13.1	ug/l	155885	3	10.055	593552	50.0
Propanoic acid,...	9.482	51.5	ug/l	611966	3	10.055	593552	50.0
Acetic acid, bu...	9.580	34.1	ug/l	405380	3	10.055	593552	50.0
Isopropyl butyrate	9.915	92.0	ug/l	1092480	3	10.055	593552	50.0
Butanoic acid, ...	10.640	8.6	ug/l	101512	3	10.055	593552	50.0