

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
 Data File : VX036846.D
 Acq On : 07 Aug 2023 18:53
 Operator : JC/MD
 Sample : 03887-11
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MCLEAN-TP2

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\82X072123W.M
 Title : SW846 8260

Signal : TIC: VX036846.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.380	207	212	223	rVB	30273	50920	2.80%	0.460%
2	2.788	273	279	295	rVB2	10284	22669	1.25%	0.205%
3	3.331	360	368	379	rBV2	7853	18897	1.04%	0.171%
4	3.575	400	408	423	rBV	18418	44942	2.47%	0.406%
5	4.568	563	571	586	rBV3	9718	30119	1.66%	0.272%
6	5.385	692	705	721	rBV2	92138	269673	14.83%	2.435%
7	5.556	721	733	748	rVV	146741	420430	23.12%	3.796%
8	5.958	788	799	815	rBV	97587	262165	14.41%	2.367%
9	6.342	851	862	879	rBV	79562	208168	11.45%	1.879%
10	6.763	921	931	944	rBV	243189	589901	32.43%	5.326%
11	7.641	1069	1075	1080	rBV	48535	88029	4.84%	0.795%
12	7.696	1080	1084	1093	rVB	14967	28127	1.55%	0.254%
13	7.799	1093	1101	1122	rBV	1073762	1818772	100.00%	16.421%
14	8.549	1216	1224	1234	rBV2	244157	485521	26.69%	4.383%
15	8.647	1234	1240	1249	rBV	496812	806708	44.35%	7.283%
16	8.952	1284	1290	1307	rBV	296920	439678	24.17%	3.970%
17	9.244	1332	1338	1344	rBV	307434	429273	23.60%	3.876%
18	9.311	1344	1349	1351	rVV	31428	45647	2.51%	0.412%
19	9.348	1351	1355	1356	rVV	50392	67588	3.72%	0.610%
20	9.378	1356	1360	1367	rVB	127750	184812	10.16%	1.669%
21	9.482	1372	1377	1383	rBV	573440	725880	39.91%	6.554%
22	9.580	1388	1393	1405	rVB	391273	495405	27.24%	4.473%
23	9.915	1442	1448	1461	rBV	1017164	1287338	70.78%	11.623%
24	10.055	1463	1471	1478	rBV	536058	761502	41.87%	6.875%
25	10.281	1503	1508	1516	rBV	14062	19642	1.08%	0.177%
26	10.506	1541	1545	1558	rVB	17058	22011	1.21%	0.199%
27	10.640	1562	1567	1578	rVB	89966	112451	6.18%	1.015%
28	11.079	1634	1639	1652	rBV	459700	571845	31.44%	5.163%
29	11.555	1713	1717	1724	rBV	14978	18583	1.02%	0.168%
30	12.024	1788	1794	1805	rBV	554212	710263	39.05%	6.413%
31	12.219	1821	1826	1837	rBV	24061	39161	2.15%	0.354%

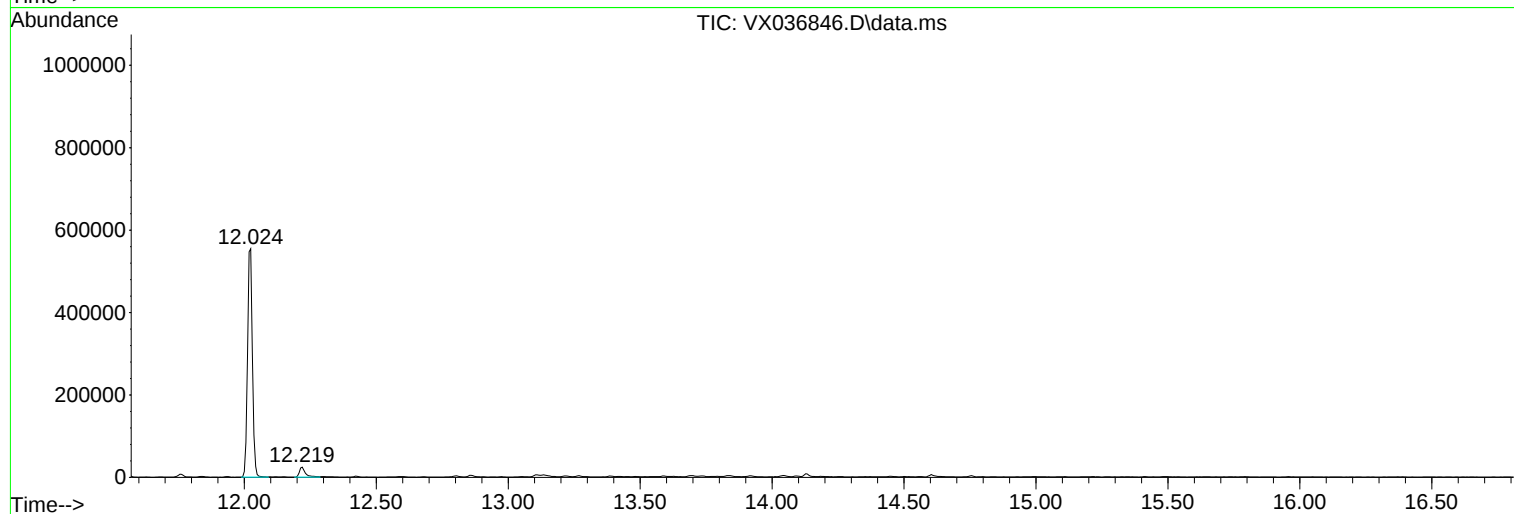
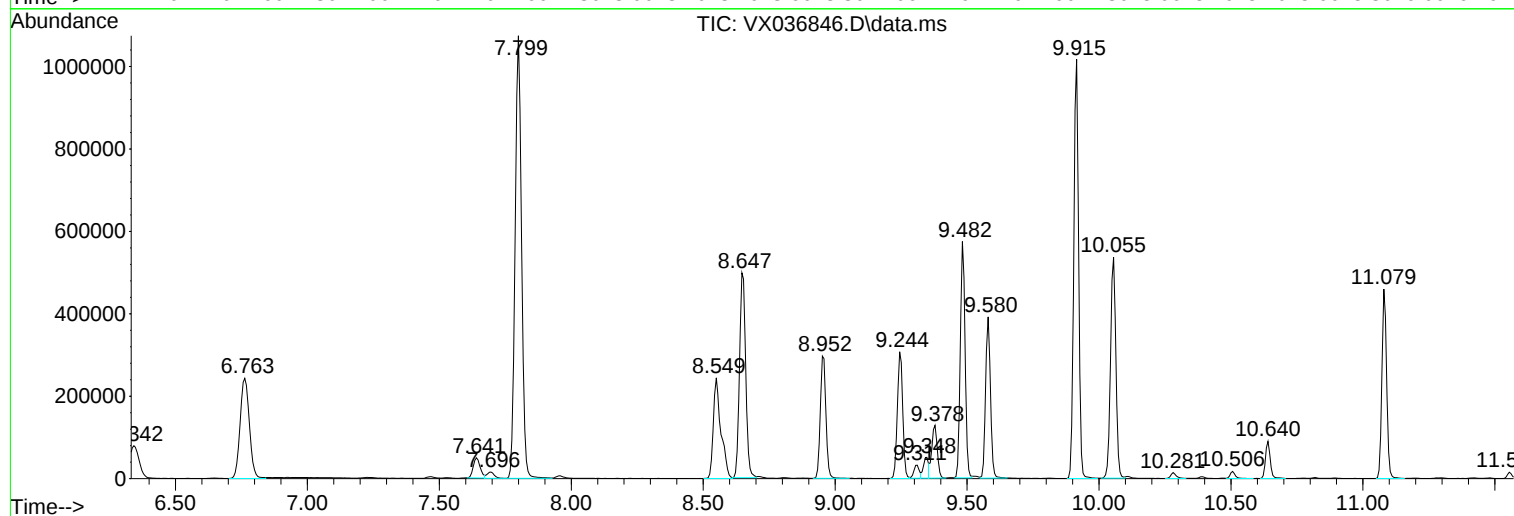
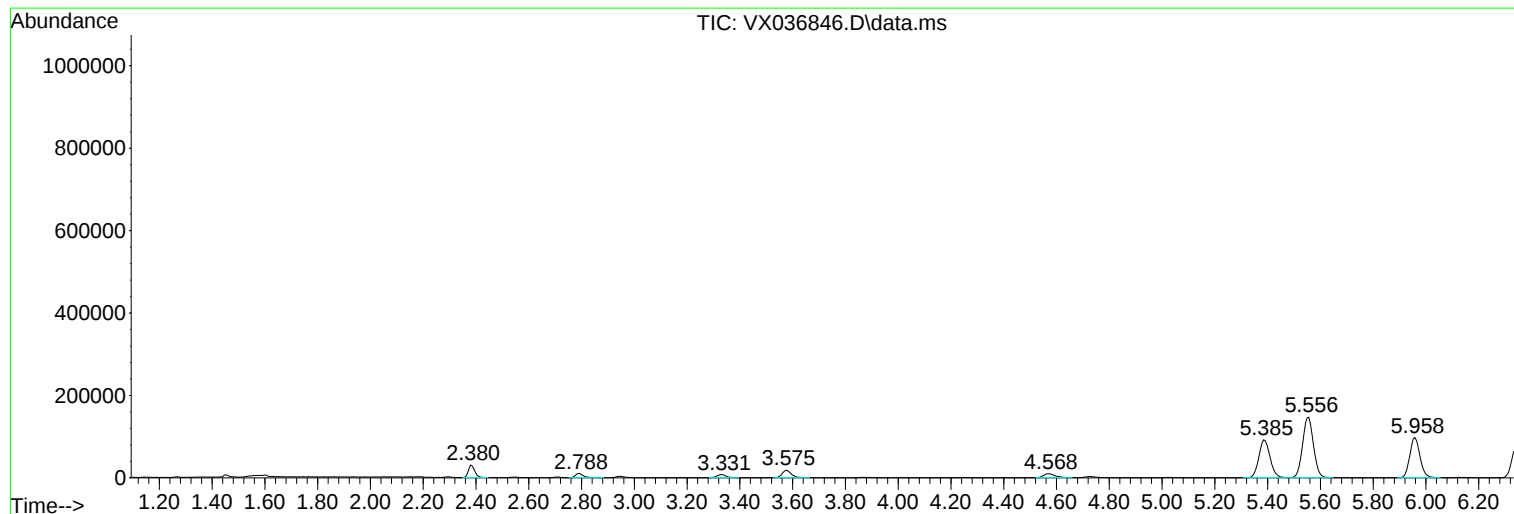
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ClientSampleId :
MCLEAN-TP2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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



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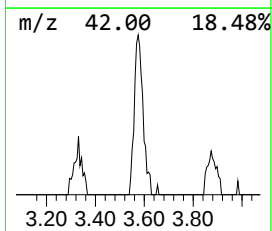
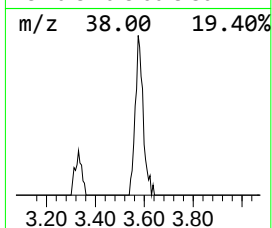
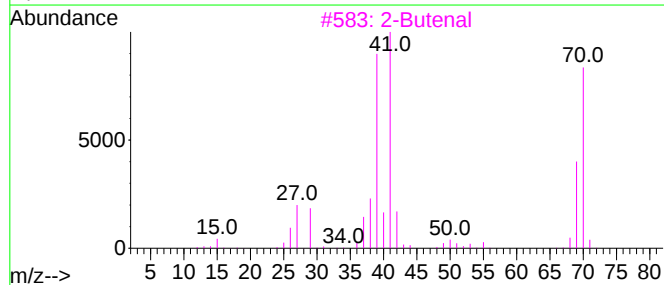
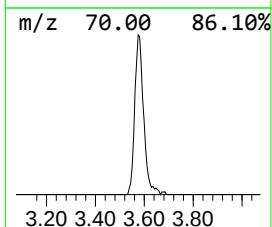
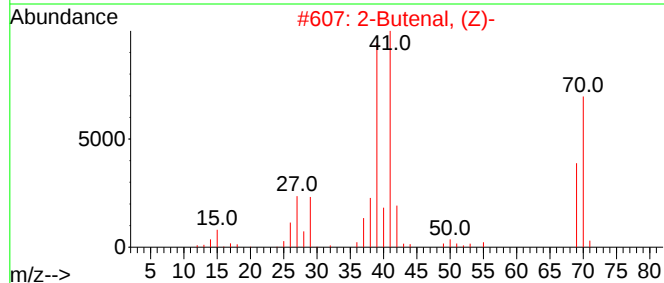
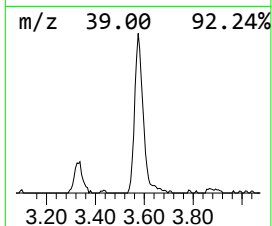
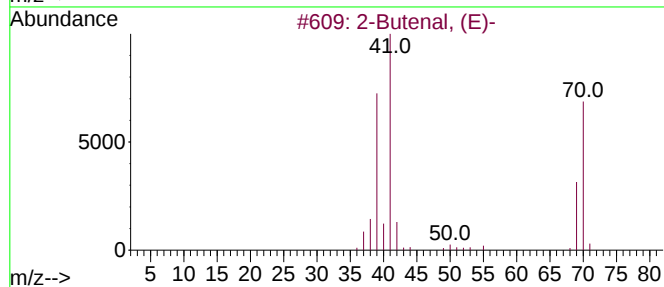
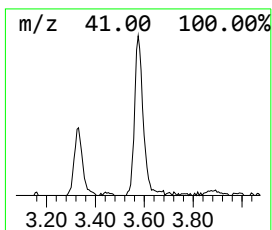
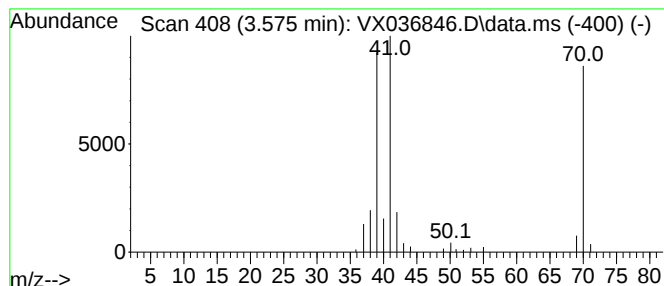
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 1 2-Butenal, (E)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.575	5.34 ug/l	44942	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenal, (E)-			70	C4H6O	000123-73-9	91
2	2-Butenal, (Z)-			70	C4H6O	015798-64-8	91
3	2-Butenal			70	C4H6O	004170-30-3	91
4	Methacrolein			70	C4H6O	000078-85-3	91
5	Furan, 2,3-dihydro-			70	C4H6O	001191-99-7	91



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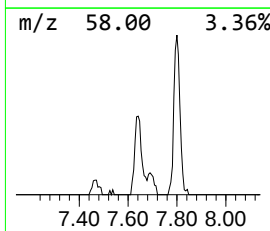
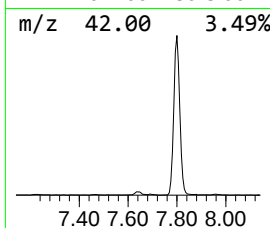
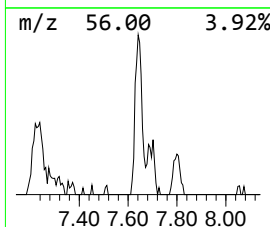
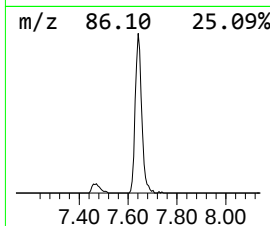
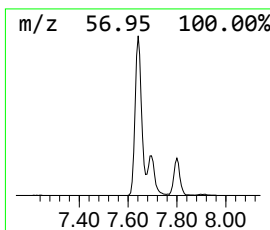
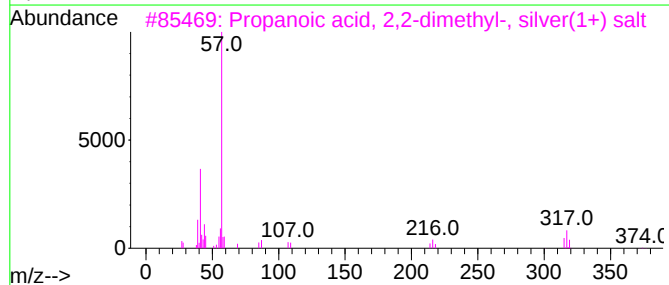
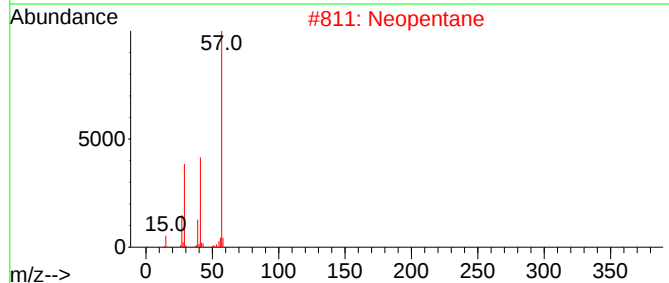
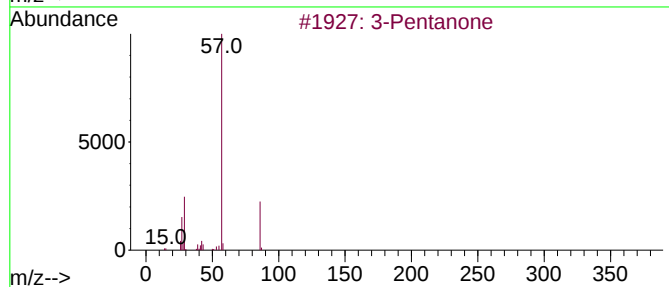
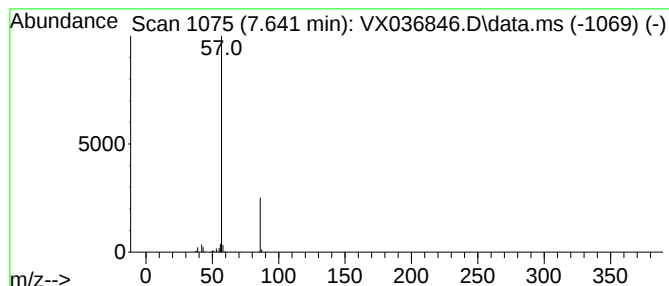
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 2 3-Pentanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.641	7.46 ug/l	88029	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone	86	C5H10O	000096-22-0	80
2			Neopentane	72	C5H12	000463-82-1	9
3			Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	9
4			Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	7
5			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	7



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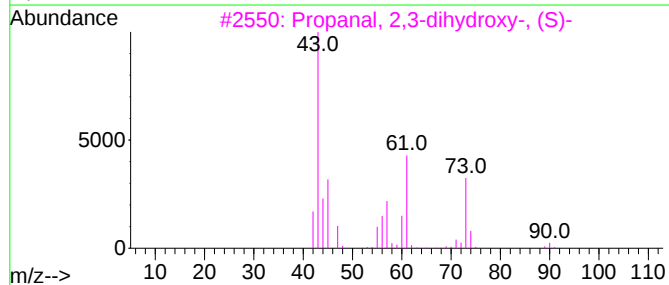
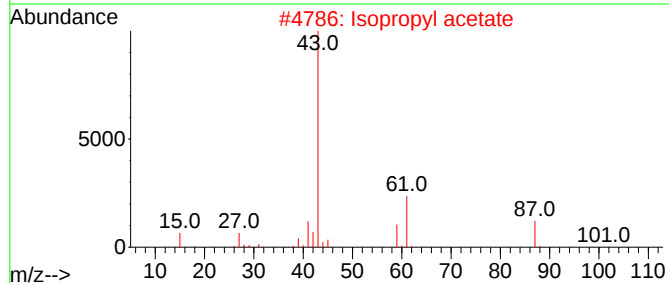
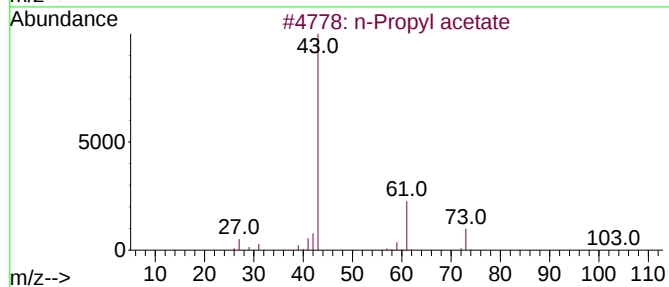
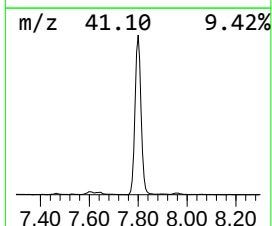
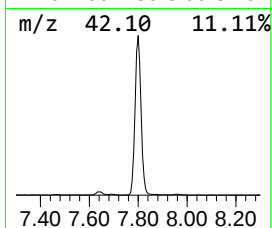
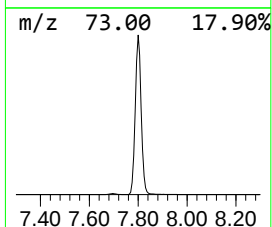
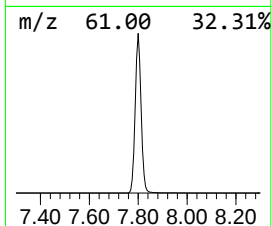
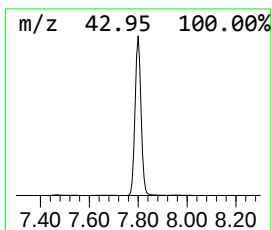
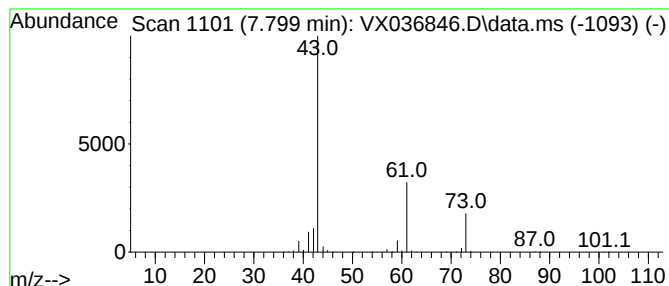
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	154.16 ug/l	1818770	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		Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	9
4		Isobutyl acetate	116	C6H12O2	000110-19-0	9
5		1-Butanamine	73	C4H11N	000109-73-9	7



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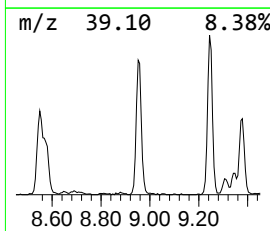
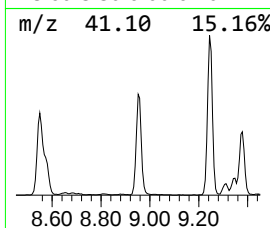
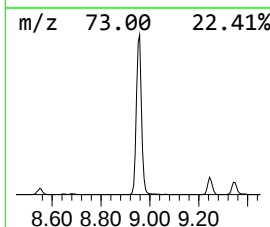
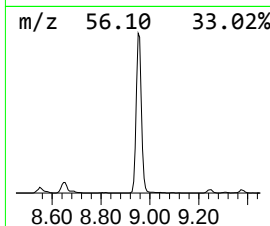
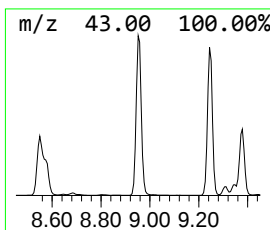
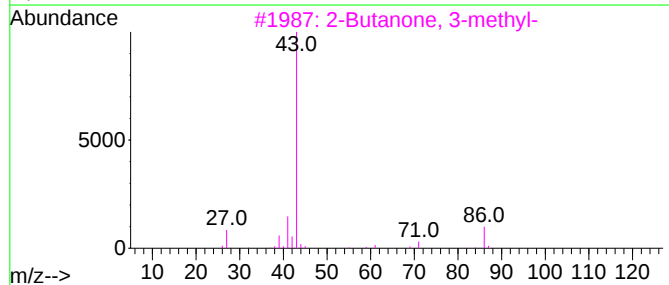
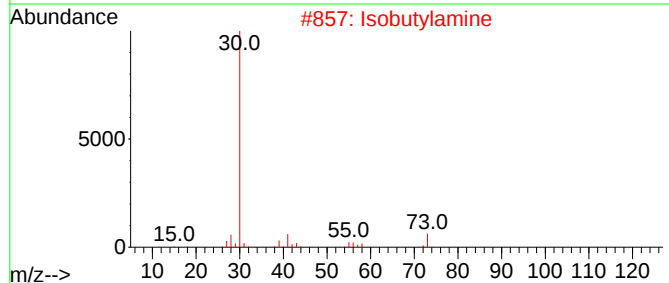
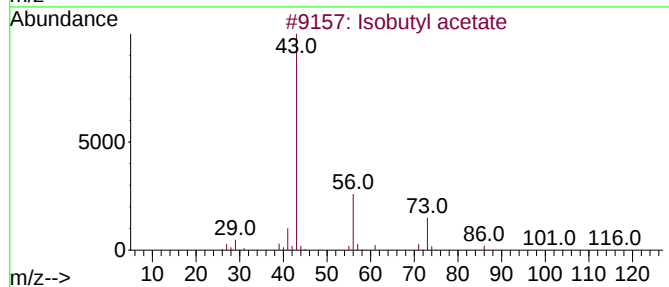
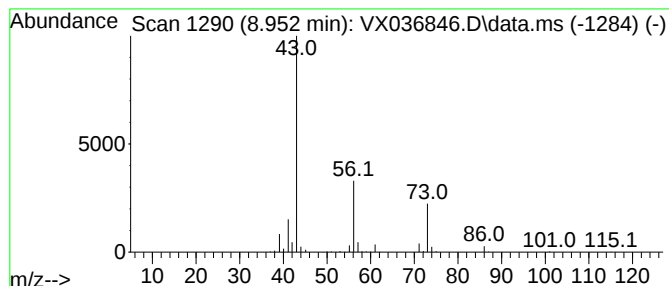
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Peak Number 4 Isobutyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.952	28.87 ug/l	439678	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutyl acetate	116	C6H12O2	000110-19-0	83
2			Isobutylamine	73	C4H11N	000078-81-9	9
3			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	9
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9
5			Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	9



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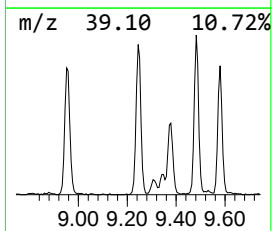
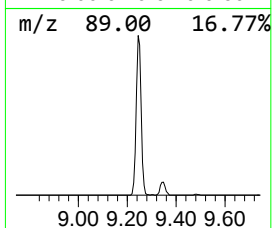
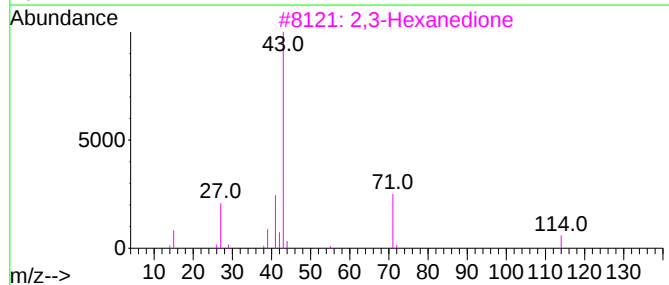
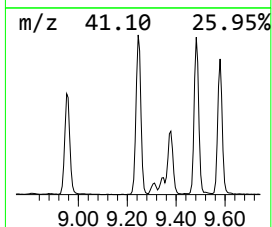
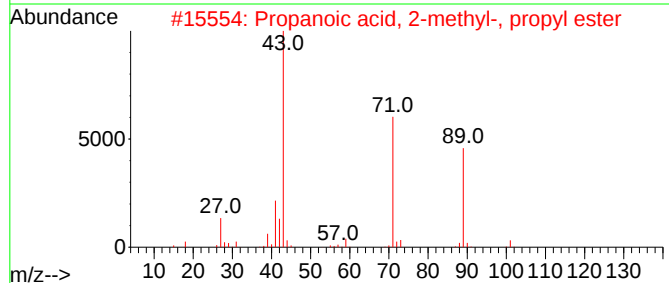
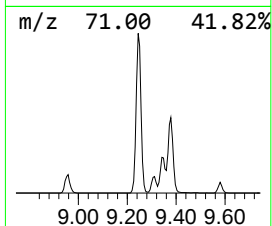
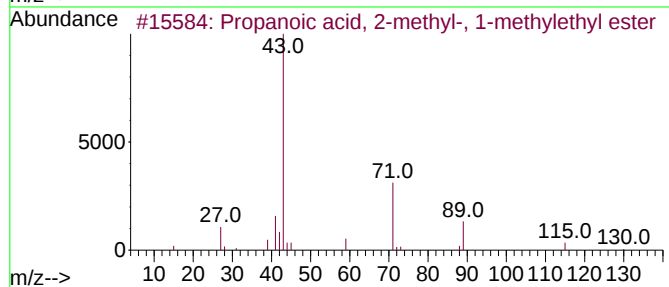
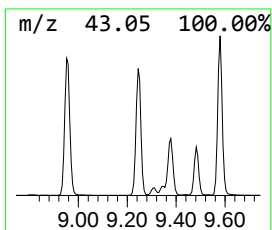
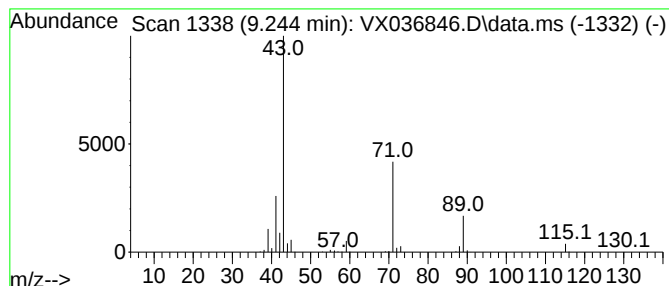
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Quant Title : SW846 8260

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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	28.19 ug/l	429273	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	72
3			2,3-Hexanedione	114	C6H10O2	003848-24-6	53
4			Isopropyl butyrate	130	C7H14O2	000638-11-9	43
5			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	40



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MCLEAN-TP2

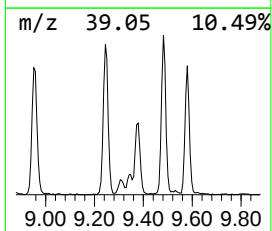
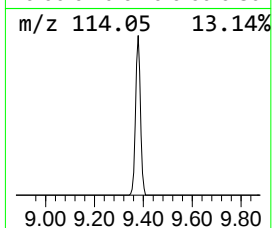
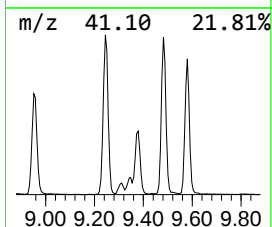
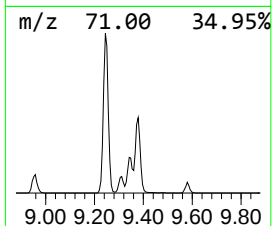
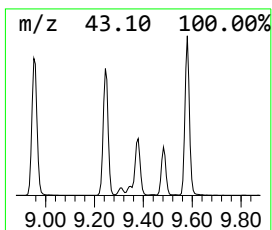
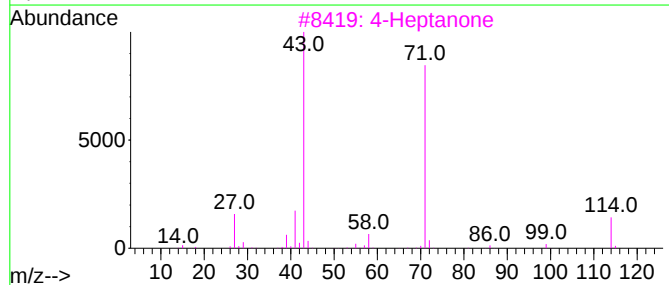
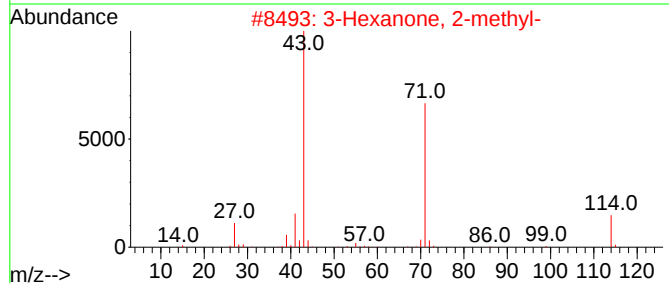
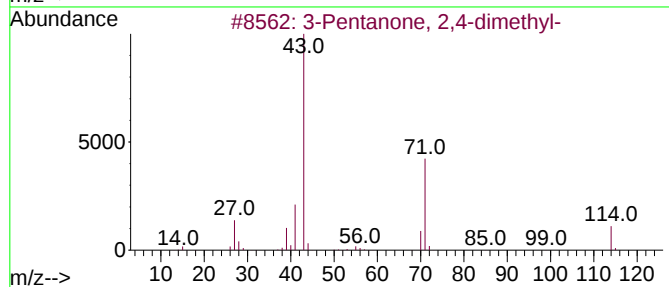
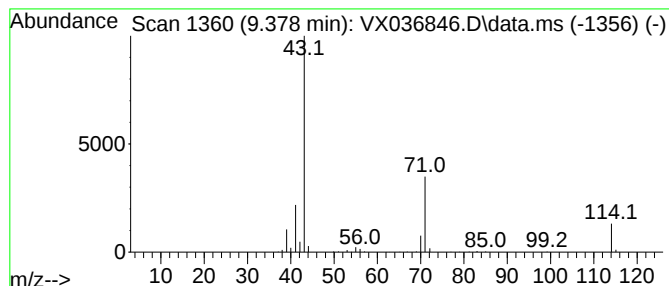
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Quant Title : SW846 8260

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

Peak Number 6 3-Pentanone, 2,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.378	12.13 ug/l	184812	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	83
2			3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	78
3			4-Heptanone	114	C7H14O	000123-19-3	64
4			2,3-Hexanedione	114	C6H10O2	003848-24-6	50
5			3,4-Dimethyl-2-pentanone	114	C7H14O	1000202-23-1	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036846.D
Acq On : 07 Aug 2023 18:53
Operator : JC/MD
Sample : 03887-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MCLEAN-TP2

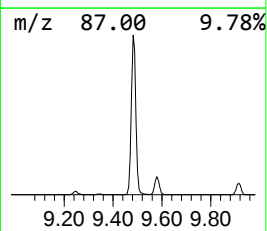
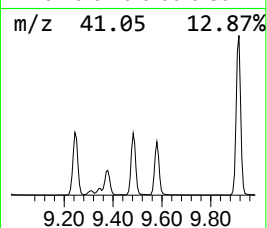
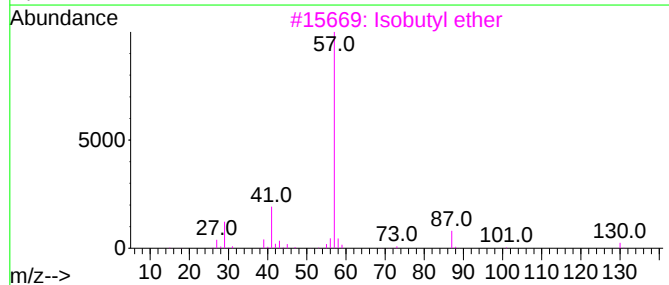
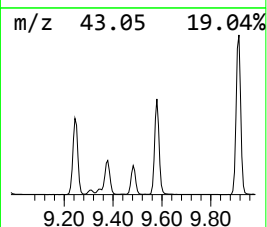
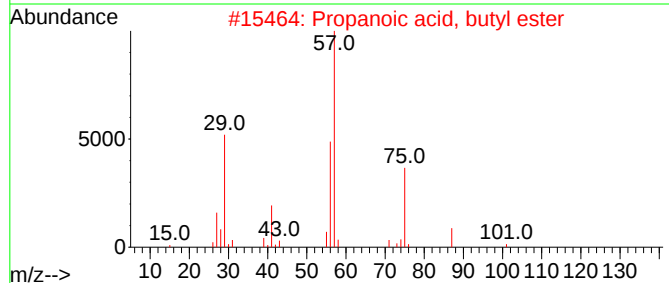
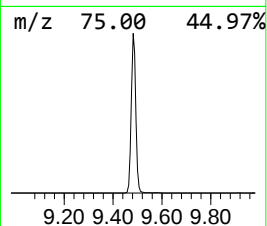
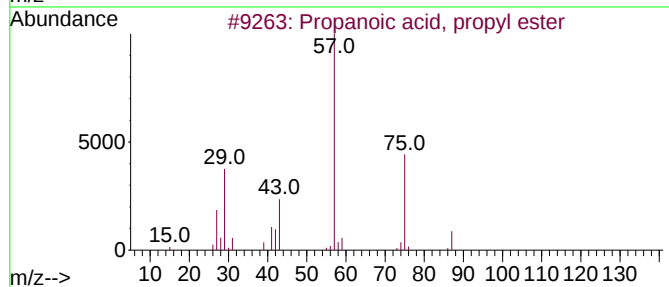
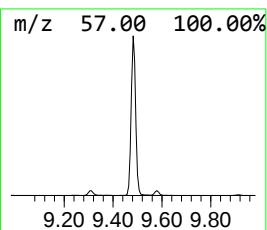
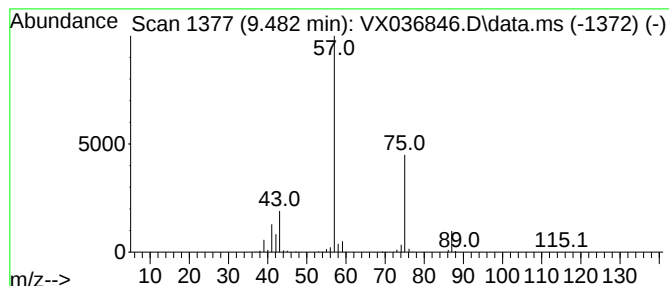
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Quant Title : SW846 8260

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	47.66 ug/l	725880	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			Isobutyl ether	130	C8H18O	000628-55-7	12
4			2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9
5			di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	8



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036846.D
Acq On : 07 Aug 2023 18:53
Operator : JC/MD
Sample : 03887-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MCLEAN-TP2

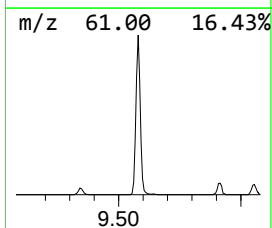
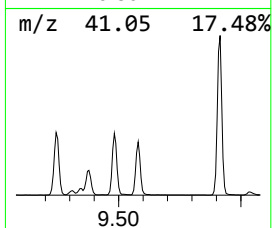
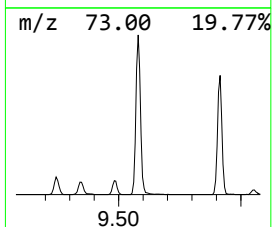
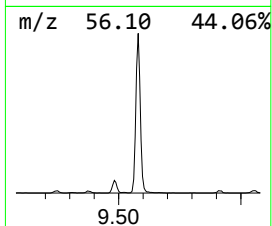
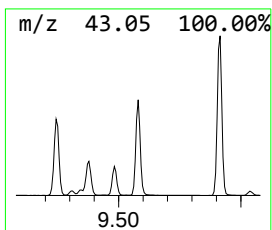
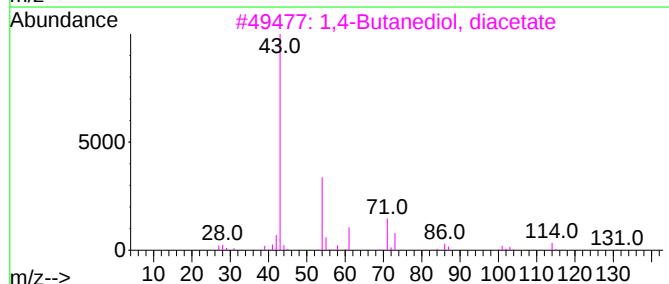
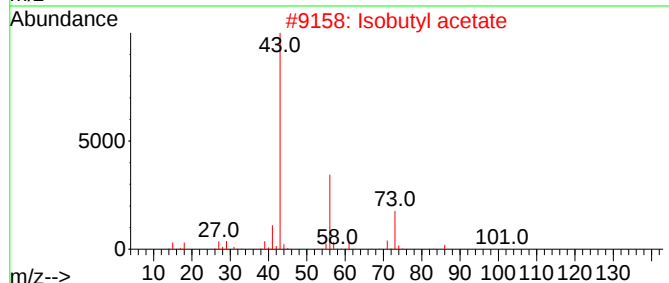
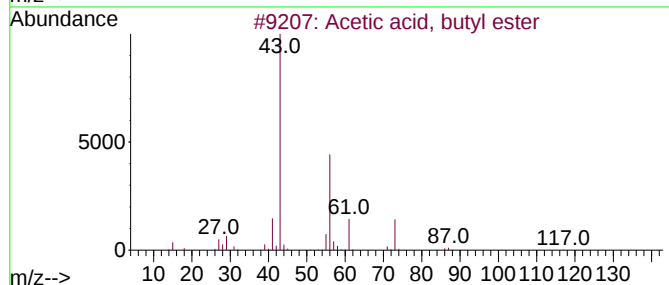
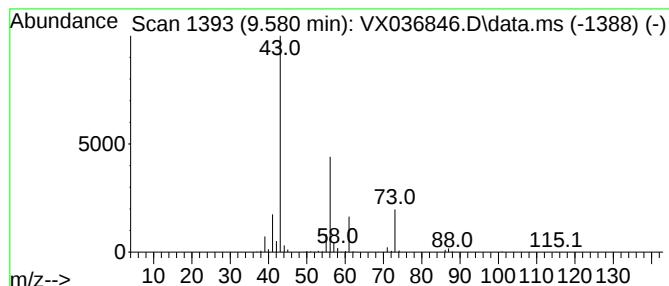
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Quant Title : SW846 8260

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	32.53 ug/l	495405	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			1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	12
4			Isobutylamine	73	C4H11N	000078-81-9	9
5			Isopropyl acetate	102	C5H10O2	000108-21-4	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036846.D
Acq On : 07 Aug 2023 18:53
Operator : JC/MD
Sample : 03887-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MCLEAN-TP2

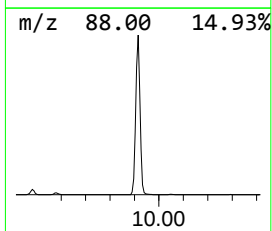
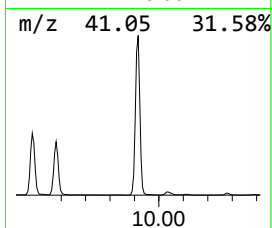
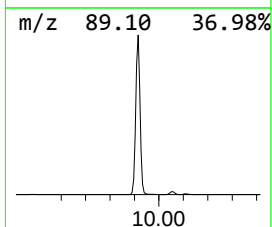
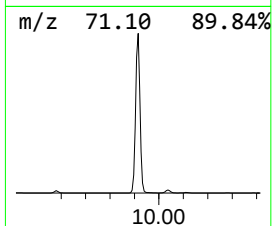
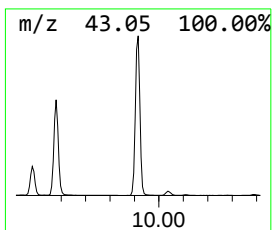
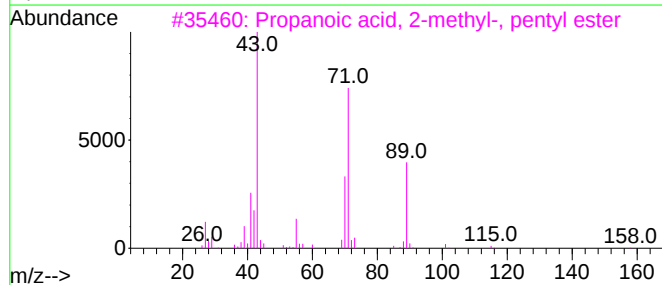
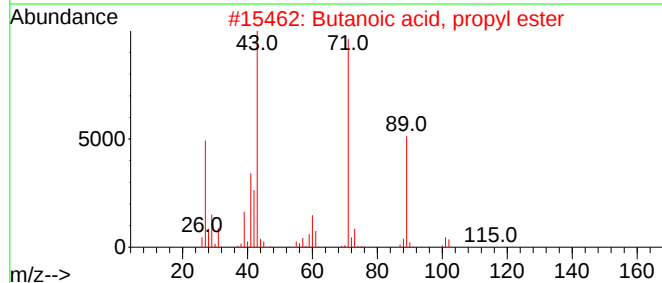
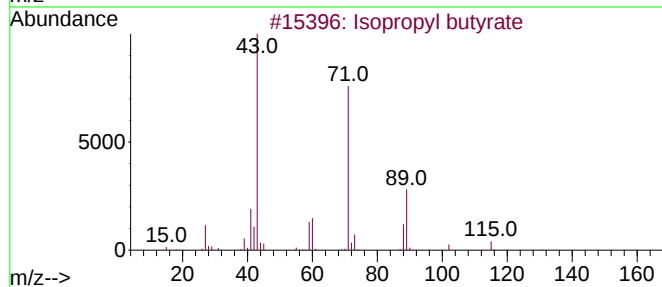
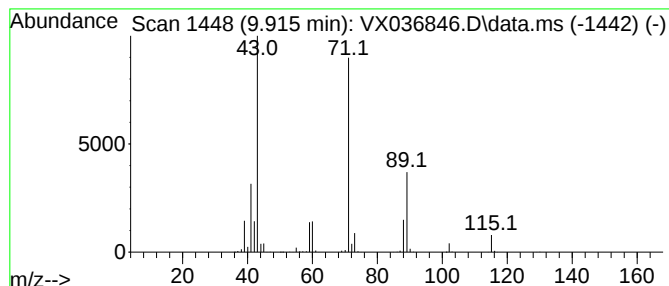
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Quant Title : SW846 8260

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	84.53 ug/l	1287340	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
3			Propanoic acid, 2-methyl-, pentyl...	158	C9H18O2	002445-72-9	64
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59
5			Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036846.D
Acq On : 07 Aug 2023 18:53
Operator : JC/MD
Sample : 03887-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MCLEAN-TP2

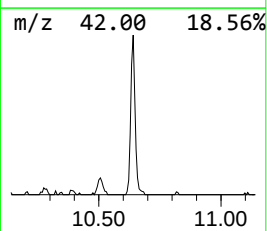
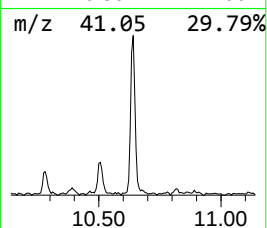
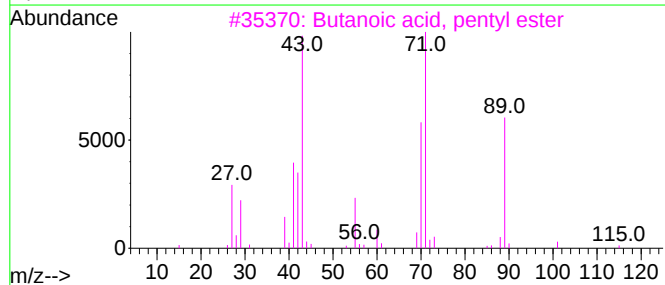
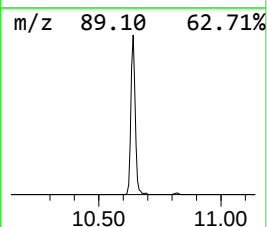
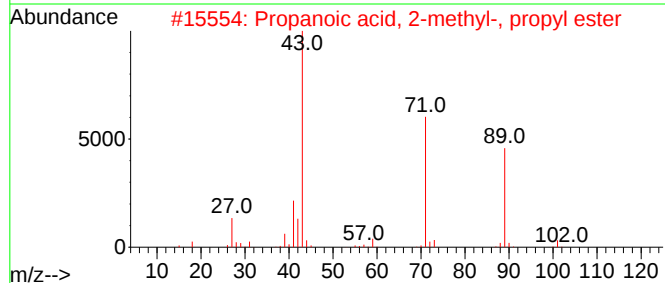
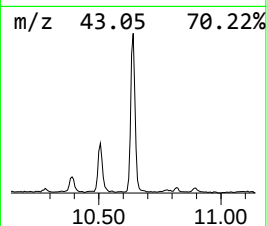
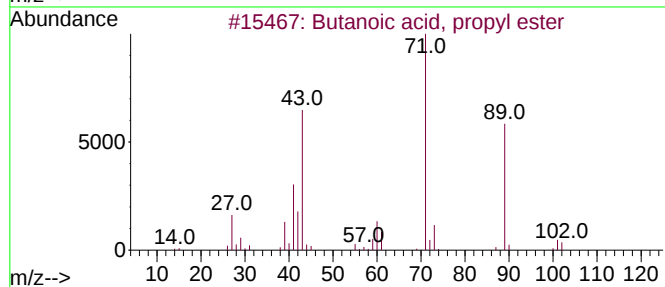
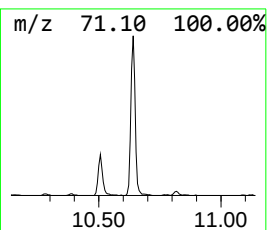
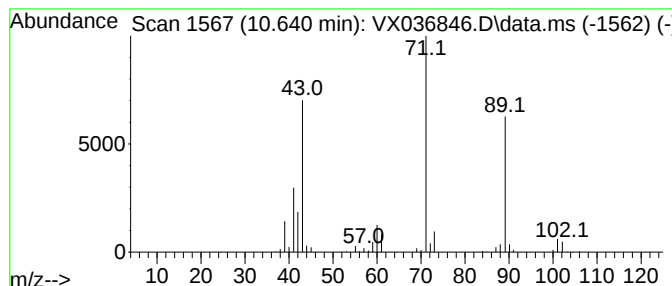
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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	7.38 ug/l	112451	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			Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	72
3			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
4			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	50
5			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036846.D
Acq On : 07 Aug 2023 18:53
Operator : JC/MD
Sample : 03887-11
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MCLEAN-TP2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.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
2-Butenal, (E)-	3.575	5.3	ug/l	44942	1	5.556	420430	50.0
3-Pentanone	7.641	7.5	ug/l	88029	2	6.763	589901	50.0
n-Propyl acetate	7.799	154.2	ug/l	1818770	2	6.763	589901	50.0
Isobutyl acetate	8.952	28.9	ug/l	439678	3	10.055	761502	50.0
Propanoic acid,...	9.244	28.2	ug/l	429273	3	10.055	761502	50.0
3-Pentanone, 2,...	9.378	12.1	ug/l	184812	3	10.055	761502	50.0
Propanoic acid,...	9.482	47.7	ug/l	725880	3	10.055	761502	50.0
Acetic acid, bu...	9.580	32.5	ug/l	495405	3	10.055	761502	50.0
Isopropyl butyrate	9.915	84.5	ug/l	1287340	3	10.055	761502	50.0
Butanoic acid, ...	10.640	7.4	ug/l	112451	3	10.055	761502	50.0