

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
 Data File : VX036845.D
 Acq On : 07 Aug 2023 18:29
 Operator : JC/MD
 Sample : 03895-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MCLEAN-TP11

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: VX036845.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.587	69	82	93	rBV10	4660	19271	1.05%	0.177%
2	2.380	206	212	223	rBV	34551	59121	3.22%	0.543%
3	2.788	271	279	295	rBV	24329	51632	2.81%	0.474%
4	3.331	358	368	377	rBV	8330	19336	1.05%	0.178%
5	3.581	399	409	420	rBV4	12088	29664	1.61%	0.272%
6	4.568	563	571	586	rBV2	10716	33185	1.81%	0.305%
7	5.391	693	706	722	rBV2	83745	250405	13.62%	2.300%
8	5.556	722	733	752	rVB	138769	390661	21.25%	3.588%
9	5.958	789	799	813	rBV	91097	242588	13.20%	2.228%
10	6.342	853	862	881	rBV	80826	206422	11.23%	1.896%
11	6.763	921	931	945	rBV	227714	540690	29.42%	4.965%
12	7.641	1064	1075	1080	rBV	52224	95928	5.22%	0.881%
13	7.696	1080	1084	1093	rVB2	14983	27993	1.52%	0.257%
14	7.799	1093	1101	1115	rBV	1073027	1838023	100.00%	16.880%
15	8.549	1214	1224	1234	rBV2	248745	494741	26.92%	4.544%
16	8.647	1234	1240	1249	rBV	474272	744994	40.53%	6.842%
17	8.952	1284	1290	1308	rBV	302163	441988	24.05%	4.059%
18	9.244	1331	1338	1344	rBV	329036	446524	24.29%	4.101%
19	9.311	1344	1349	1351	rVV	32140	46695	2.54%	0.429%
20	9.342	1351	1354	1356	rVV	52546	68186	3.71%	0.626%
21	9.378	1356	1360	1366	rVB	129688	184433	10.03%	1.694%
22	9.482	1372	1377	1384	rBV	577722	740655	40.30%	6.802%
23	9.580	1388	1393	1403	rVB	398459	501833	27.30%	4.609%
24	9.915	1442	1448	1460	rBV	1040547	1318829	71.75%	12.112%
25	10.055	1463	1471	1478	rBV	505025	702092	38.20%	6.448%
26	10.281	1503	1508	1516	rBV	15057	20820	1.13%	0.191%
27	10.506	1541	1545	1554	rVB	17225	22069	1.20%	0.203%
28	10.640	1562	1567	1583	rVB	95737	121598	6.62%	1.117%
29	11.079	1634	1639	1654	rBV	399449	526273	28.63%	4.833%
30	11.555	1712	1717	1723	rBV	14543	18809	1.02%	0.173%
31	12.024	1788	1794	1804	rBV	491551	642340	34.95%	5.899%
32	12.219	1821	1826	1837	rBV	25732	41171	2.24%	0.378%

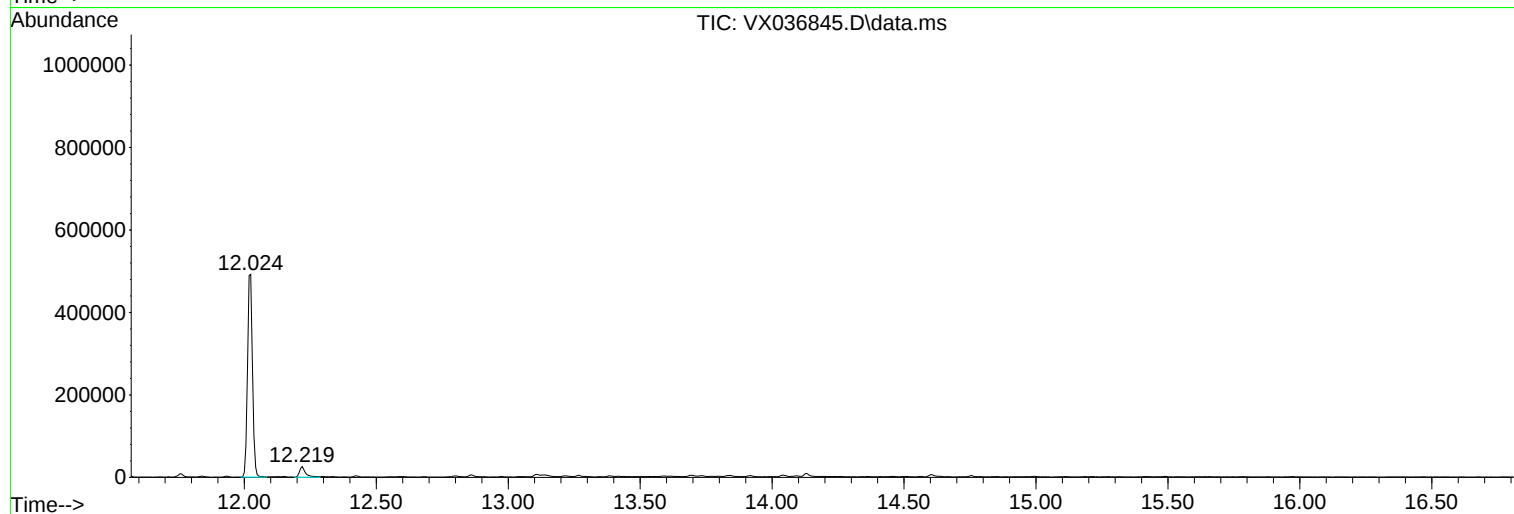
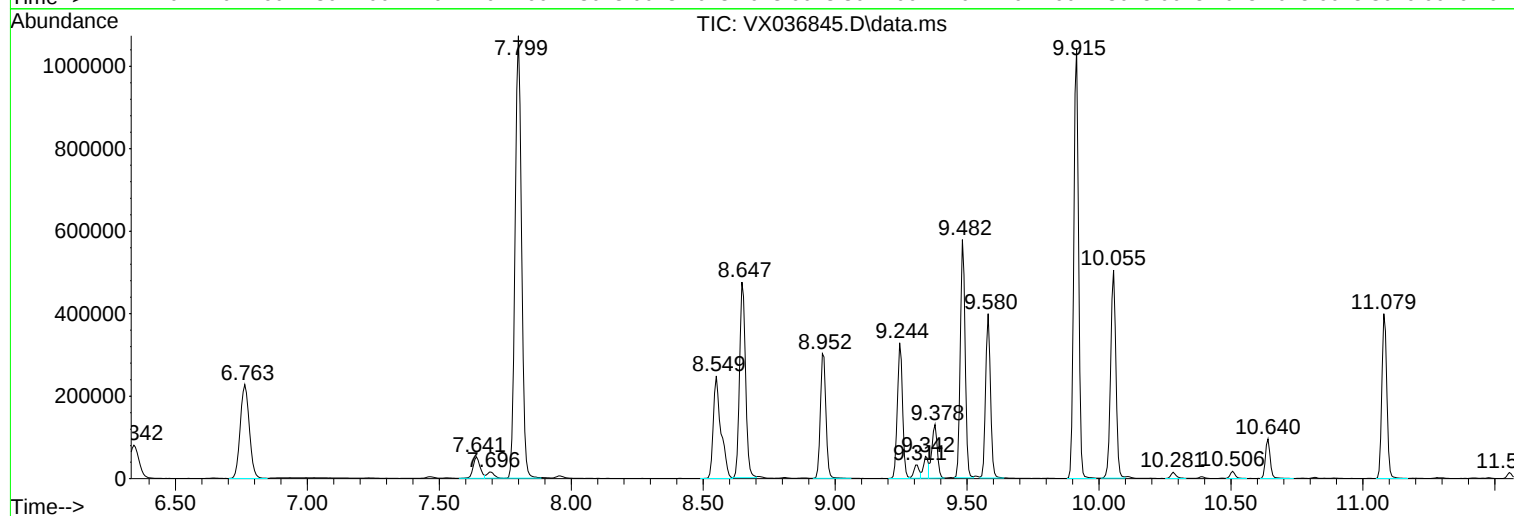
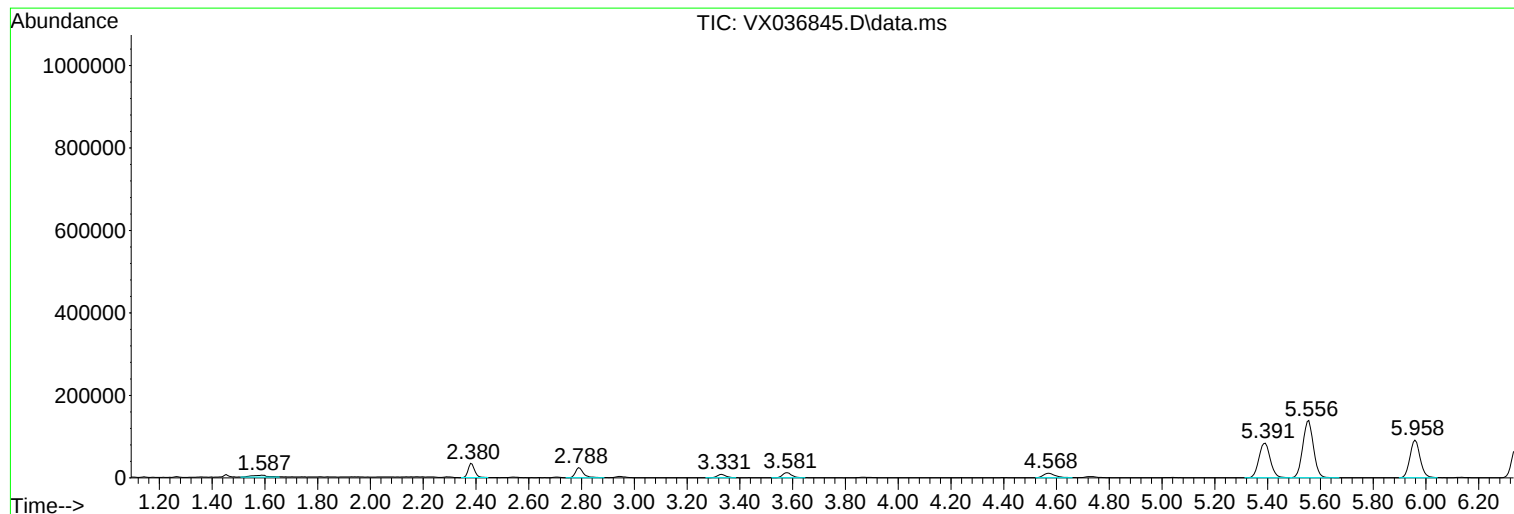
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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



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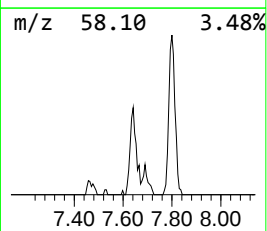
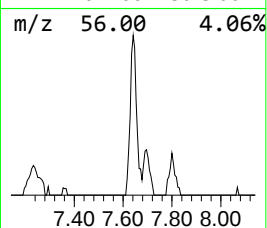
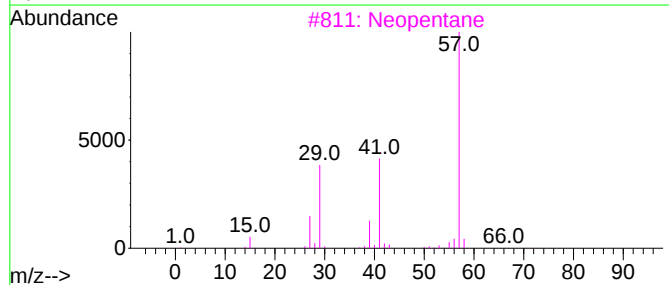
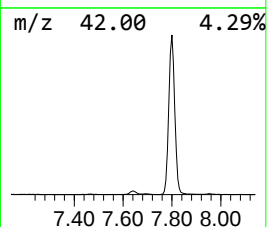
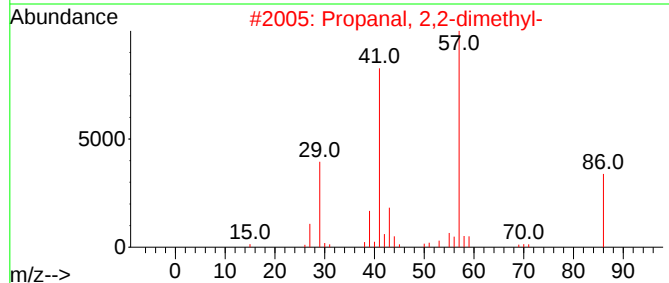
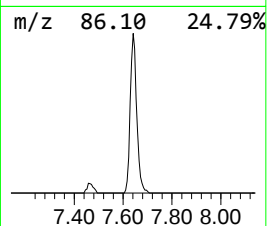
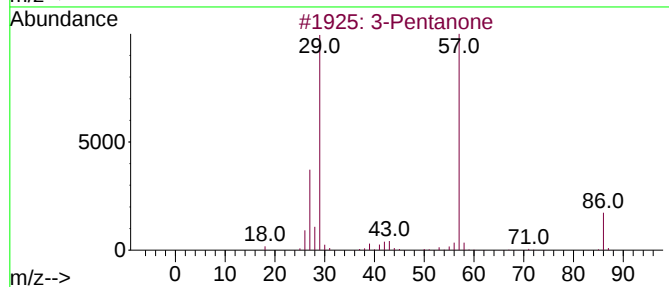
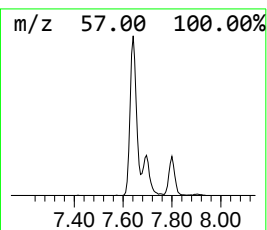
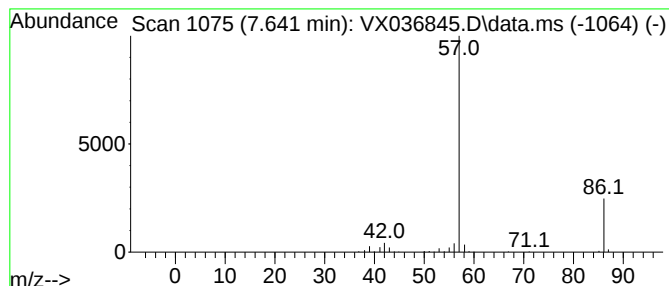
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 1 3-Pentanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.641	8.87 ug/l	95928	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone	86	C5H10O	000096-22-0	90
2			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	39
3			Neopentane	72	C5H12	000463-82-1	9
4			Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	9
5			Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	7



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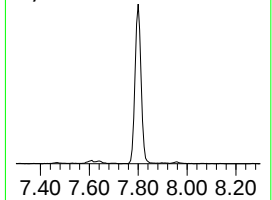
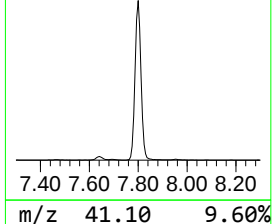
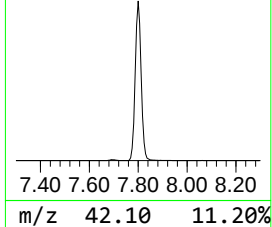
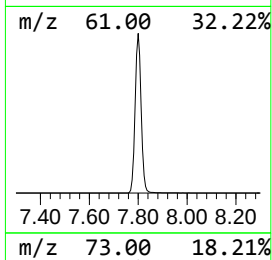
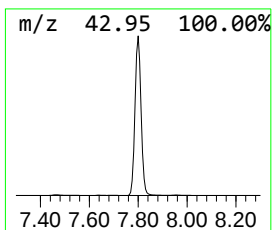
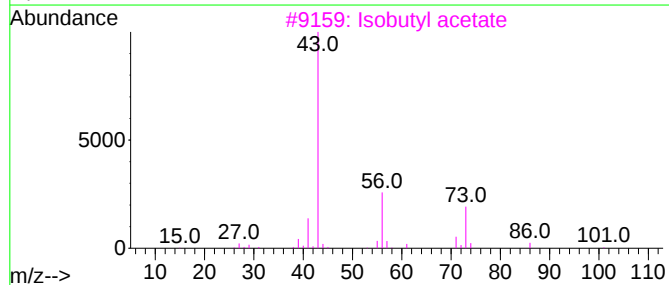
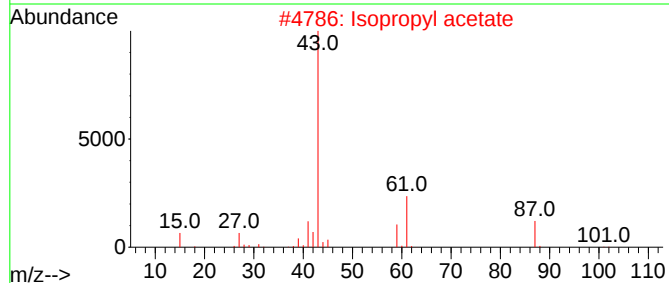
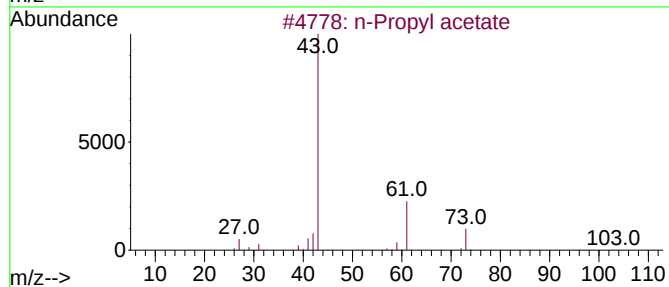
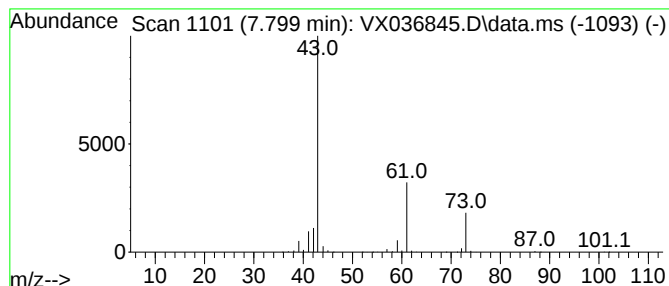
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X072123W.M
Quant Title : SW846 8260

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

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.799	169.97 ug/l	1838020	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		Isobutyl acetate	116	C6H12O2	000110-19-0	9
4		1-Butanamine	73	C4H11N	000109-73-9	7
5		Isobutylamine	73	C4H11N	000078-81-9	4



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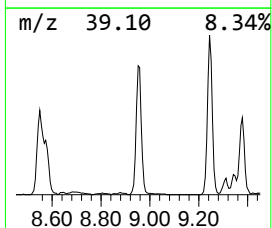
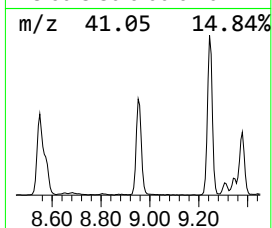
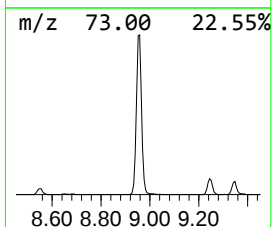
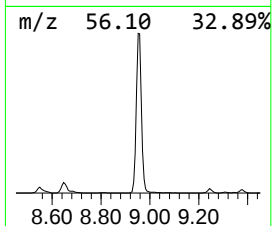
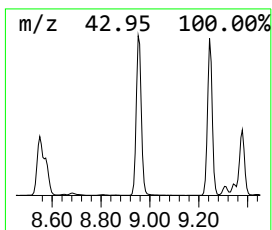
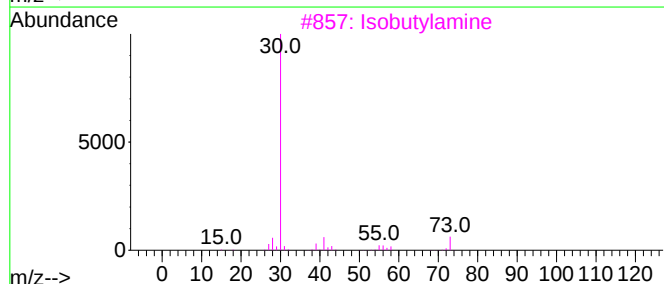
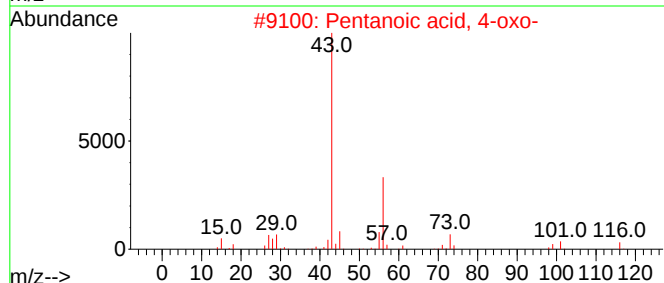
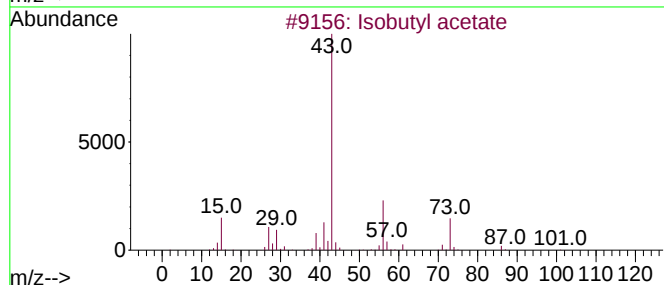
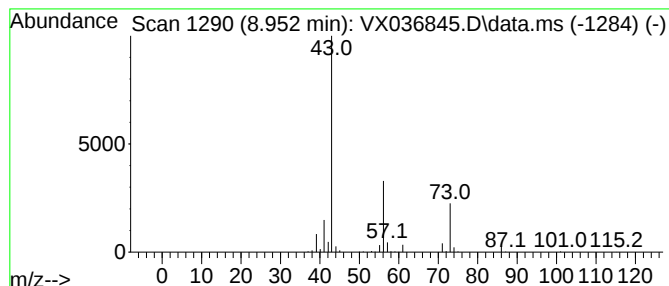
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Isobutyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.952	31.48 ug/l	441988	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutyl acetate	116	C6H12O2	000110-19-0	83
2			Pentanoic acid, 4-oxo-	116	C5H8O3	000123-76-2	38
3			Isobutylamine	73	C4H11N	000078-81-9	9
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9
5			2-Pentanone	86	C5H10O	000107-87-9	9



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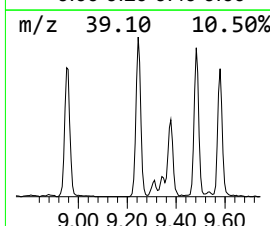
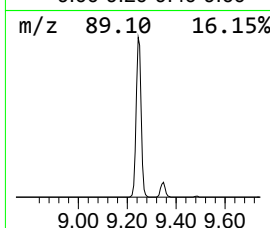
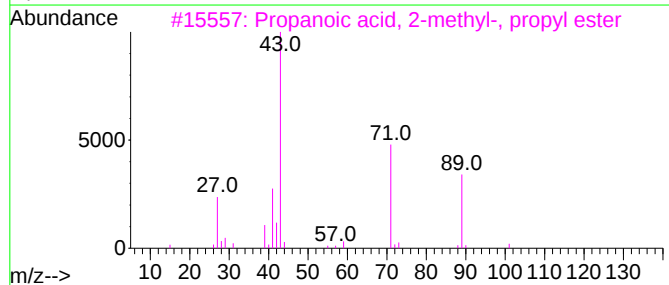
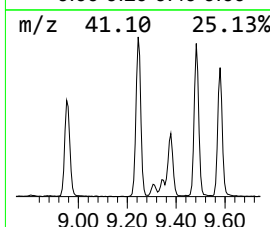
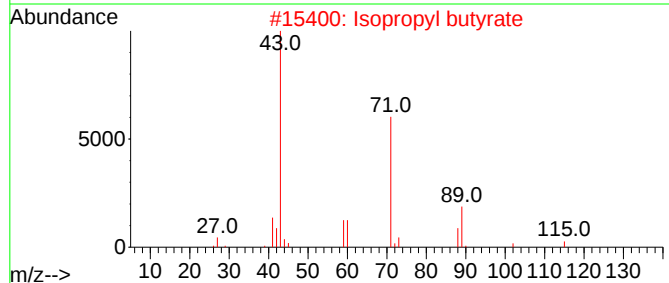
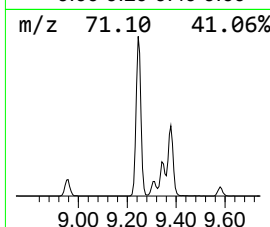
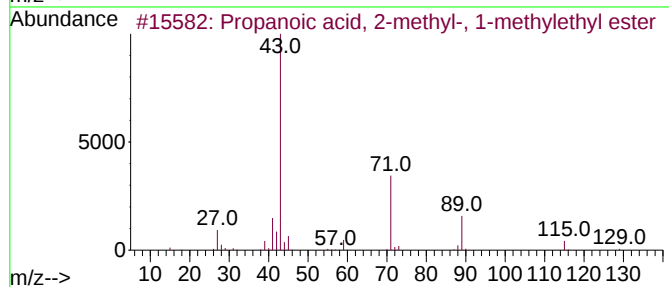
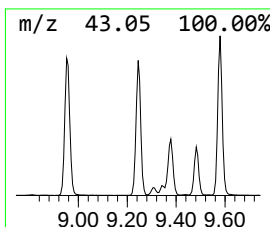
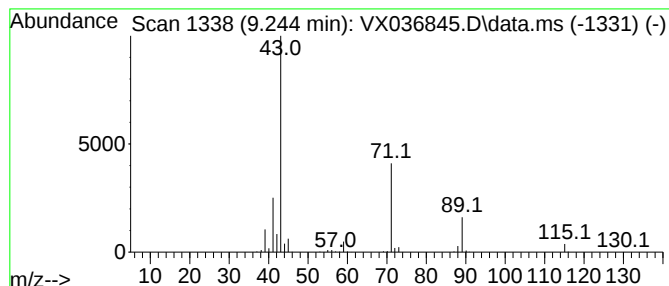
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Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.244	31.80 ug/l	446524	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			Isopropyl butyrate	130	C7H14O2	000638-11-9	72
3			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56
4			2,3-Hexanedione	114	C6H10O2	003848-24-6	42
5			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	36



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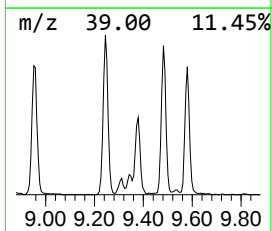
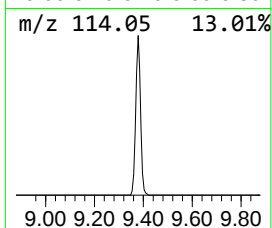
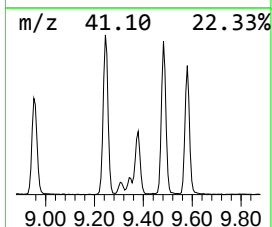
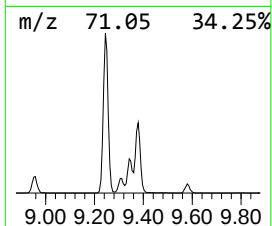
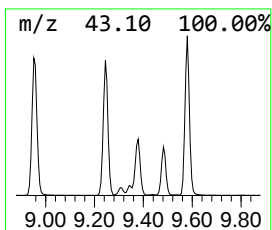
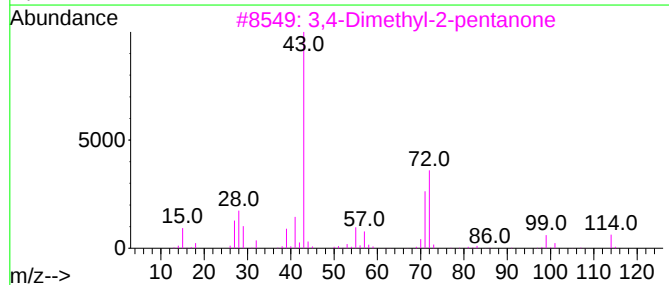
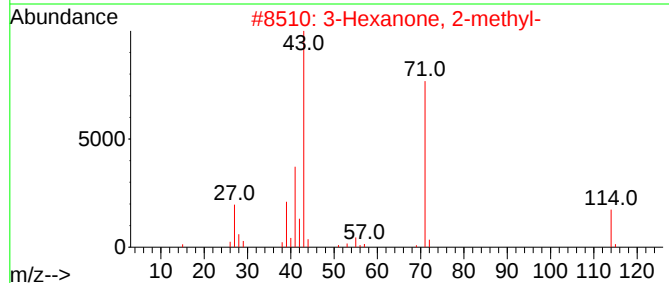
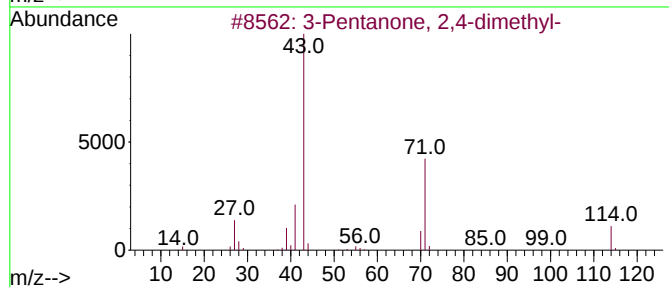
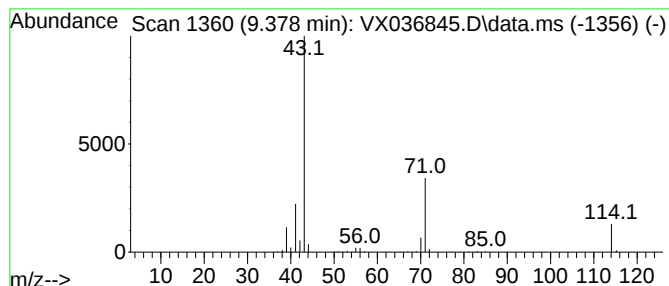
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TIC Integration Parameters: LSCINT.P

Peak Number 5 3-Pentanone, 2,4-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.378	13.13 ug/l	184433	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	80
2			3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	47
3			3,4-Dimethyl-2-pentanone	114	C7H14O	1000202-23-1	45
4			2,3-Hexanedione	114	C6H10O2	003848-24-6	42
5			4-Heptanone	114	C7H14O	000123-19-3	42



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MCLEAN-TP11

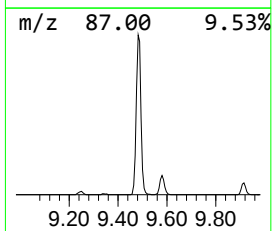
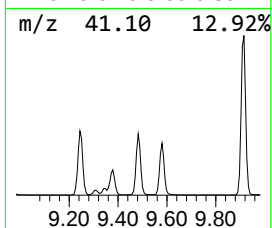
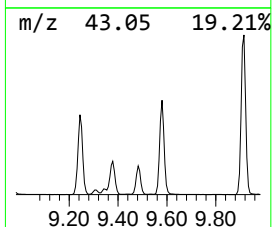
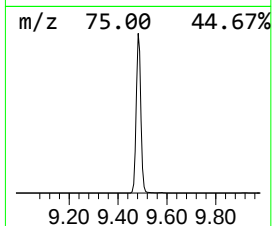
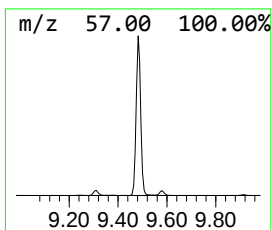
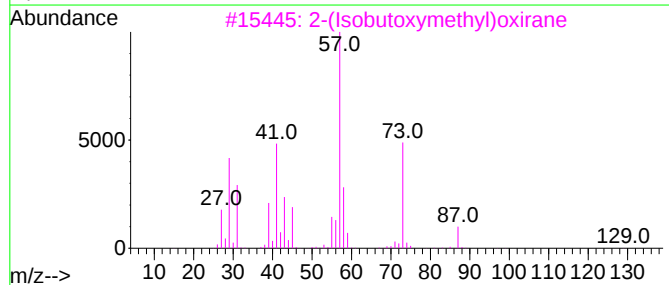
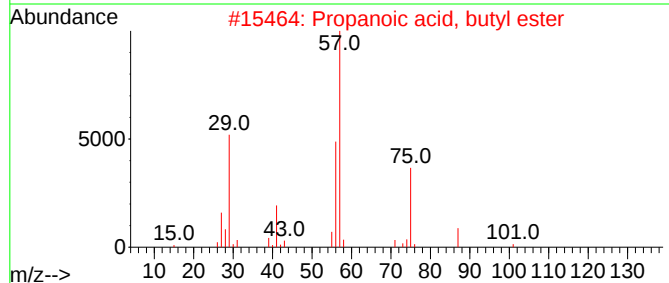
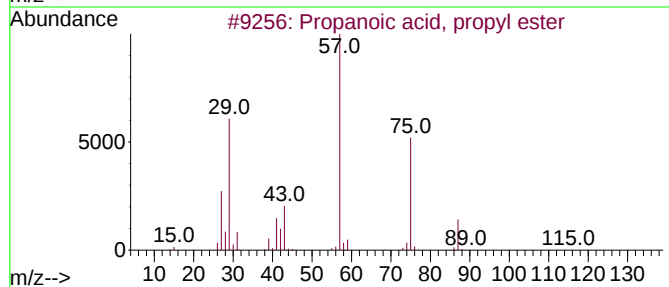
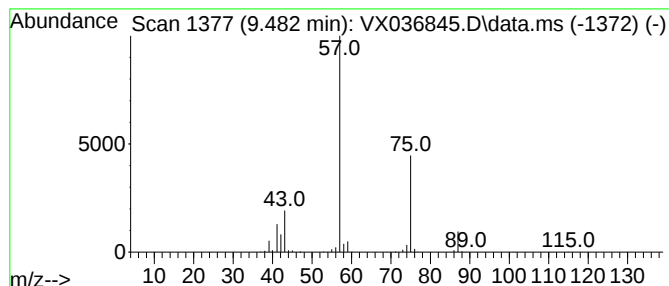
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Quant Title : SW846 8260

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

Peak Number 6 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.482	52.75 ug/l	740655	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, 2-methyl-	87	C5H13N	000096-15-1	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036845.D
Acq On : 07 Aug 2023 18:29
Operator : JC/MD
Sample : 03895-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MCLEAN-TP11

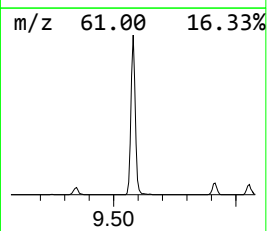
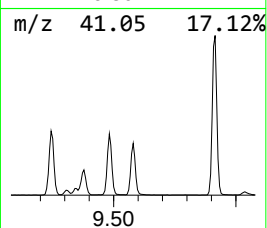
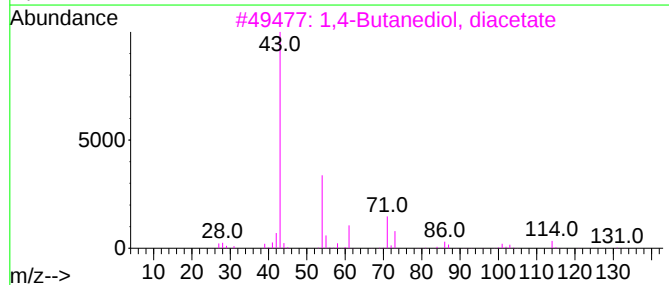
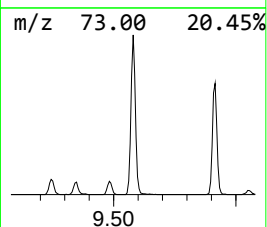
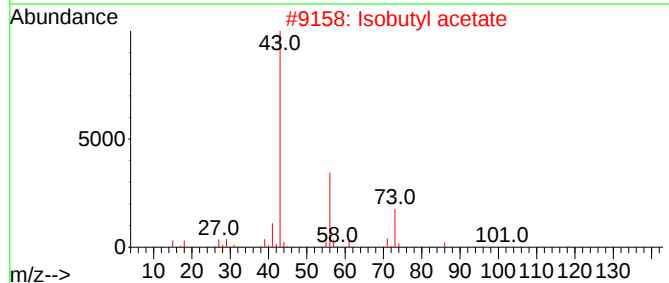
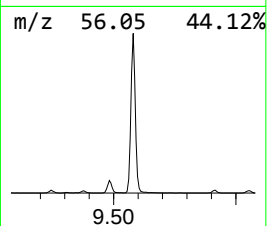
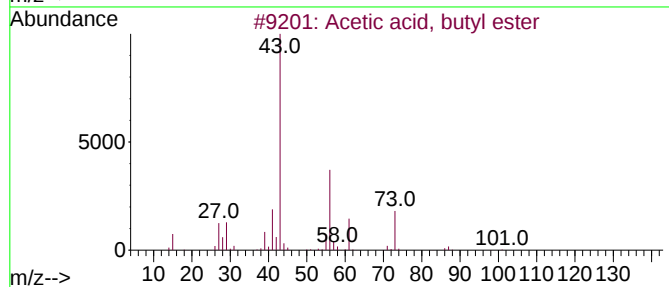
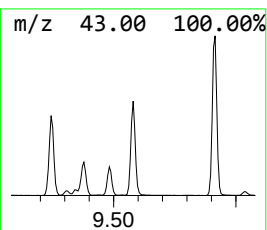
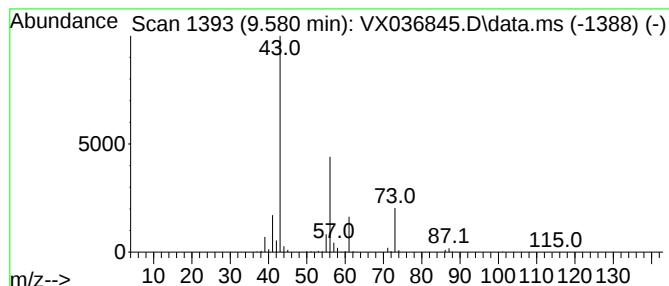
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Quant Title : SW846 8260

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

Peak Number 7 Acetic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.580	35.74 ug/l	501833	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 : VX036845.D
Acq On : 07 Aug 2023 18:29
Operator : JC/MD
Sample : 03895-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MCLEAN-TP11

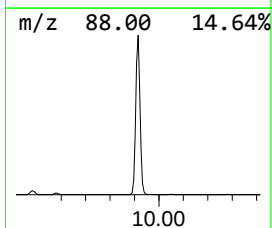
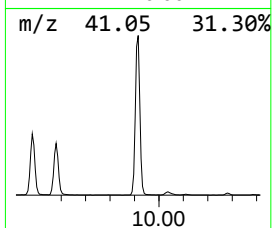
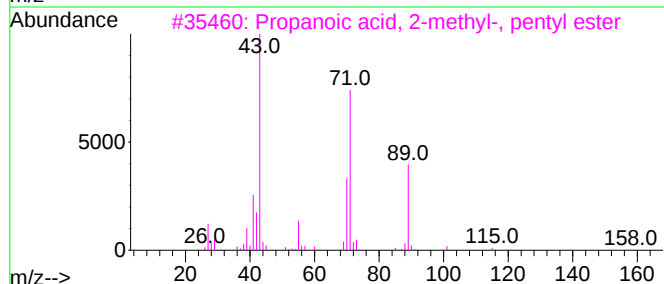
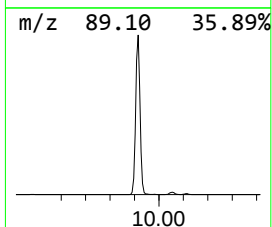
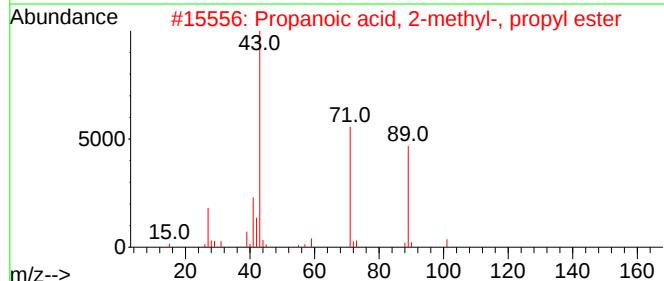
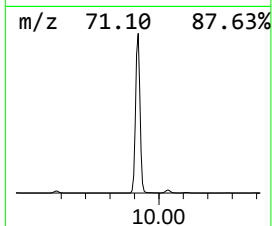
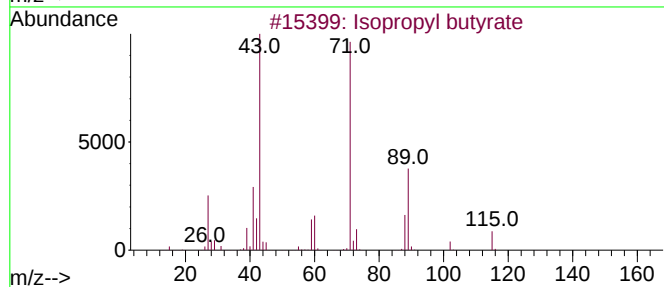
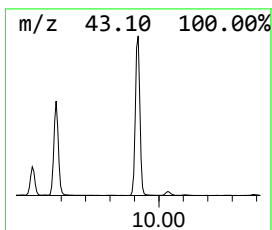
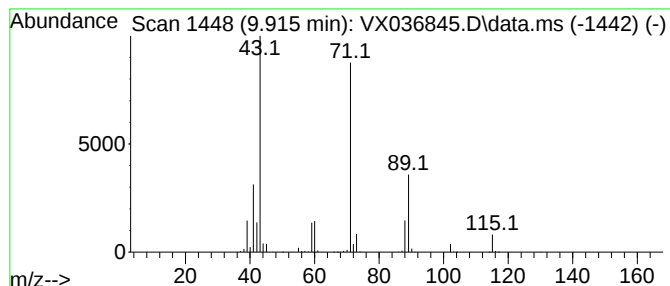
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Quant Title : SW846 8260

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

Peak Number 8 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.915	93.92 ug/l	1318830	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-, propy...	130	C7H14O2	000644-49-5	72
3			Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64
4			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	59
5			Ethane-1,1-diol dibutanoate	202	C10H18O4	025572-25-2	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036845.D
Acq On : 07 Aug 2023 18:29
Operator : JC/MD
Sample : 03895-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MCLEAN-TP11

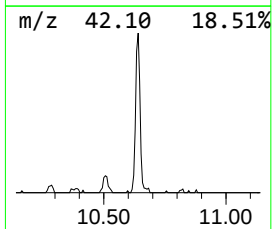
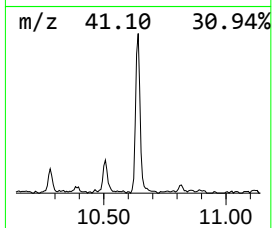
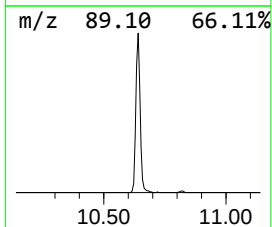
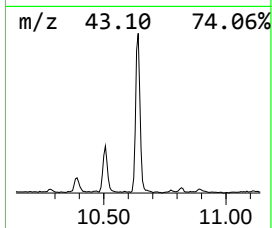
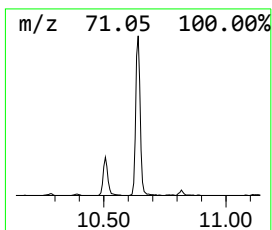
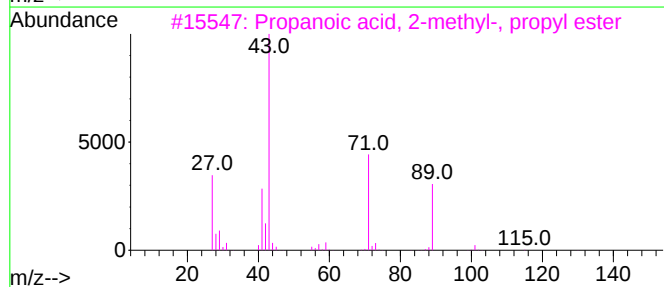
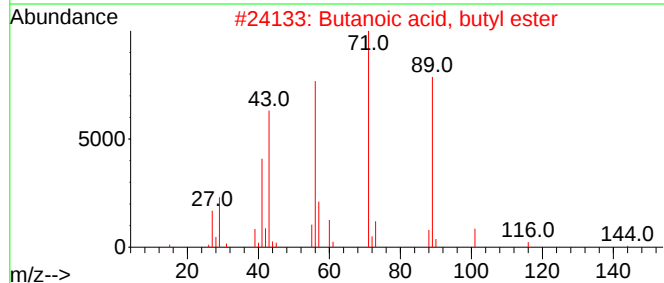
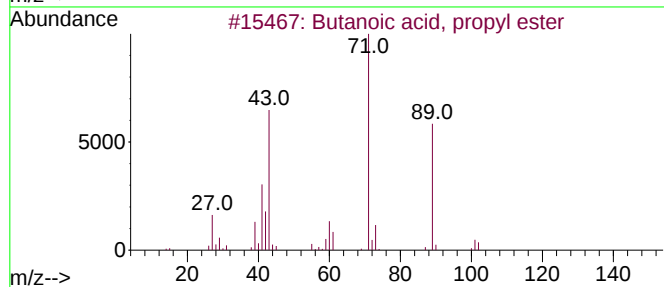
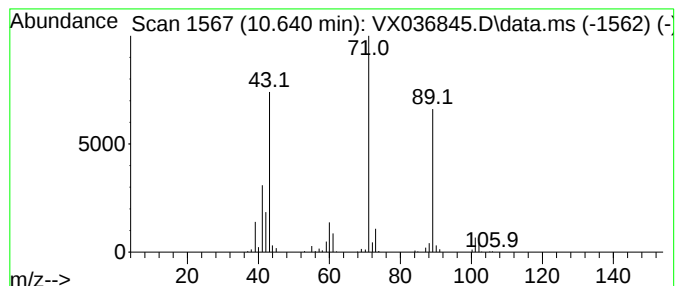
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Quant Title : SW846 8260

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

Peak Number 9 Butanoic acid, propyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.640	8.66 ug/l	121598	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, butyl ester	144	C8H16O2	000109-21-7	78
3			Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	72
4			Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
5			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX080723\
Data File : VX036845.D
Acq On : 07 Aug 2023 18:29
Operator : JC/MD
Sample : 03895-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MCLEAN-TP11

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
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n-Propyl acetate	7.799	170.0	ug/l	1838020	2	6.763	540690	50.0
Isobutyl acetate	8.952	31.5	ug/l	441988	3	10.055	702092	50.0
Propanoic acid,...	9.244	31.8	ug/l	446524	3	10.055	702092	50.0
3-Pentanone, 2,...	9.378	13.1	ug/l	184433	3	10.055	702092	50.0
Propanoic acid,...	9.482	52.8	ug/l	740655	3	10.055	702092	50.0
Acetic acid, bu...	9.580	35.7	ug/l	501833	3	10.055	702092	50.0
Isopropyl butyrate	9.915	93.9	ug/l	1318830	3	10.055	702092	50.0
Butanoic acid, ...	10.640	8.7	ug/l	121598	3	10.055	702092	50.0