

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041323\
 Data File : VN077323.D
 Acq On : 13 Apr 2023 12:58
 Operator : JC\MD
 Sample : 02292-02
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 IDW-SO-VB3-041123

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_N\methods\82N040523W.M
 Title : SW846 8260

Signal : TIC: VN077323.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.825	144	151	152	rBV2	49778	83839	1.20%	0.190%
2	5.290	559	570	584	rBV4	37253	128265	1.84%	0.290%
3	7.566	950	957	969	rVB2	57078	146956	2.11%	0.332%
4	8.172	1050	1060	1065	rBV	454684	1089903	15.63%	2.465%
5	8.231	1065	1070	1084	rVB	802306	1722624	24.70%	3.896%
6	8.583	1121	1130	1141	rBV	475948	1049741	15.05%	2.374%
7	8.695	1141	1149	1161	rBV	367787	822404	11.79%	1.860%
8	9.107	1210	1219	1230	rBV	1198010	2395999	34.35%	5.419%
9	9.672	1307	1315	1321	rBV2	172884	391809	5.62%	0.886%
10	9.748	1321	1328	1345	rVV	3870806	6974588	100.00%	15.775%
11	10.360	1422	1432	1442	rBV	879229	1507954	21.62%	3.411%
12	10.572	1459	1468	1477	rBV	1855164	3458384	49.59%	7.822%
13	10.730	1488	1495	1504	rVB	1091593	1866088	26.76%	4.221%
14	10.989	1529	1539	1548	rBV	1227673	2051604	29.42%	4.640%
15	11.083	1548	1555	1563	rVV3	232980	438917	6.29%	0.993%
16	11.207	1563	1576	1584	rVV2	1950034	3926713	56.30%	8.881%
17	11.295	1584	1591	1605	rVB	1241506	2058345	29.51%	4.655%
18	11.607	1635	1644	1657	rBV	3686716	5984761	85.81%	13.536%
19	11.771	1667	1672	1681	rVB3	56271	106206	1.52%	0.240%
20	11.871	1681	1689	1699	rVV	1641089	2960545	42.45%	6.696%
21	11.966	1699	1705	1712	rVB	48308	90062	1.29%	0.204%
22	12.213	1742	1747	1756	rVB	48280	77296	1.11%	0.175%
23	12.307	1756	1763	1774	rBV	323794	540396	7.75%	1.222%
24	12.854	1848	1856	1865	rBV	1253741	2143938	30.74%	4.849%
25	13.795	2009	2016	2026	rBV	1288185	2196743	31.50%	4.968%

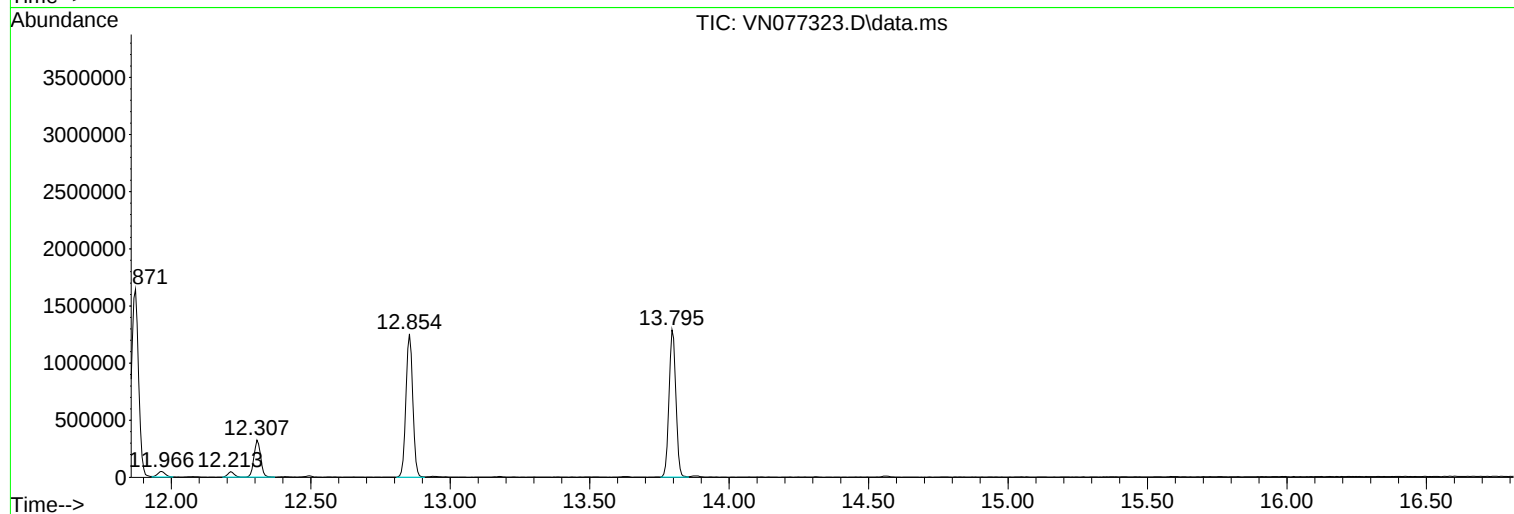
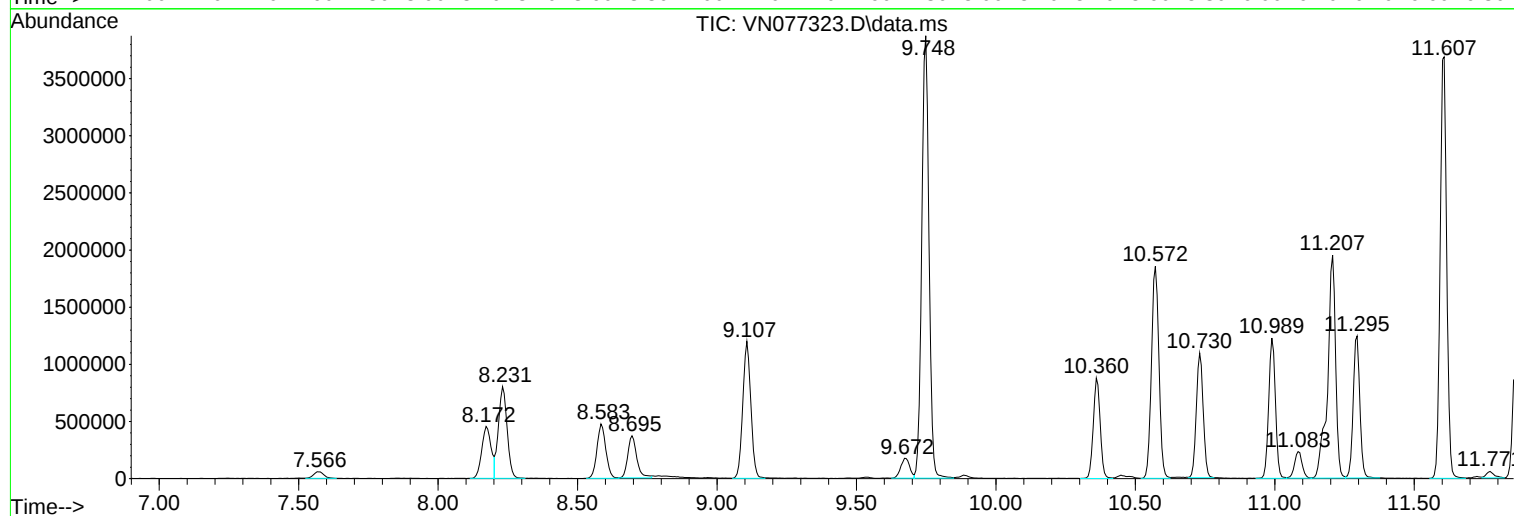
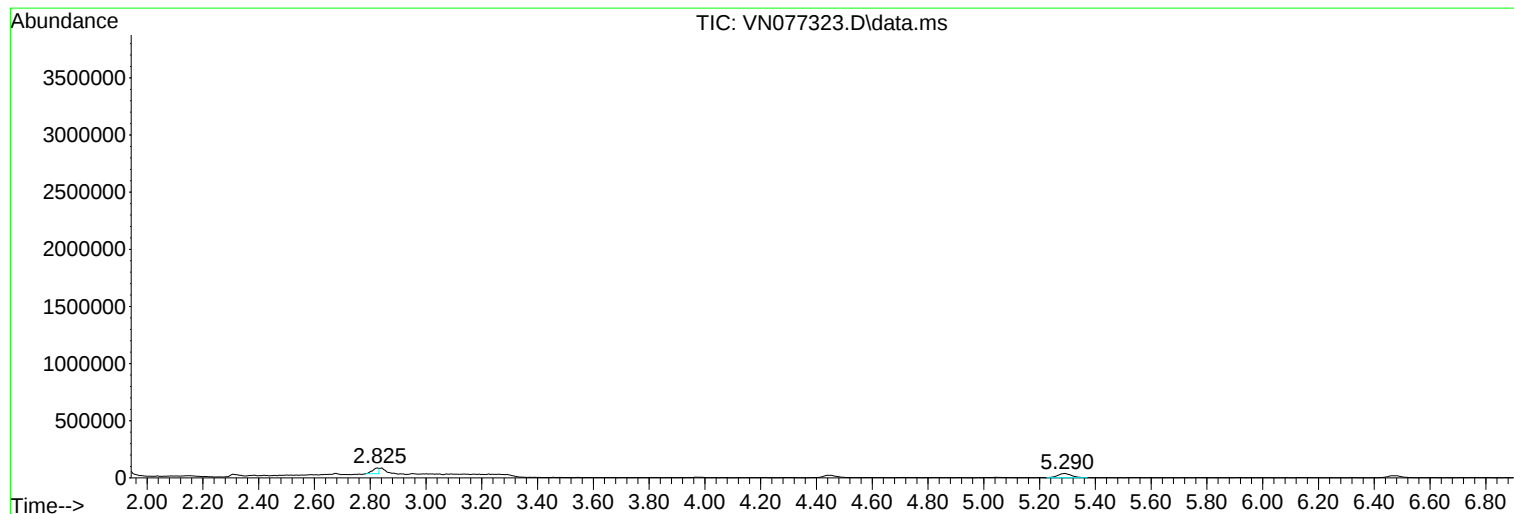
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Instrument :
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ClientSampleId :
IDW-SO-VB3-041123

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N040523W.M
Quant Title : SW846 8260

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



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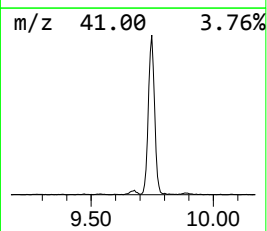
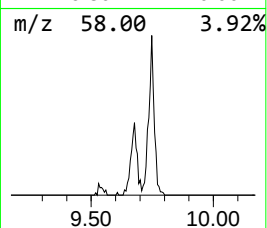
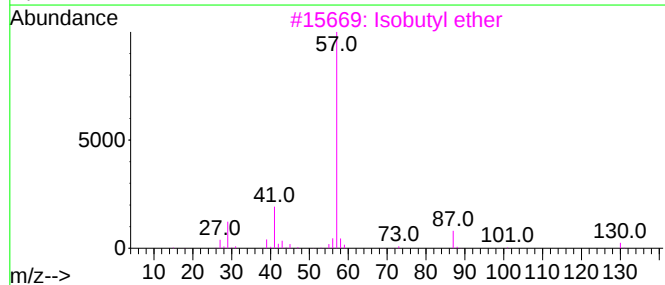
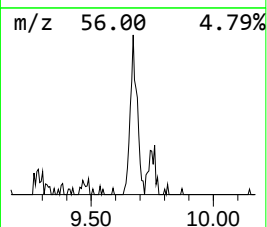
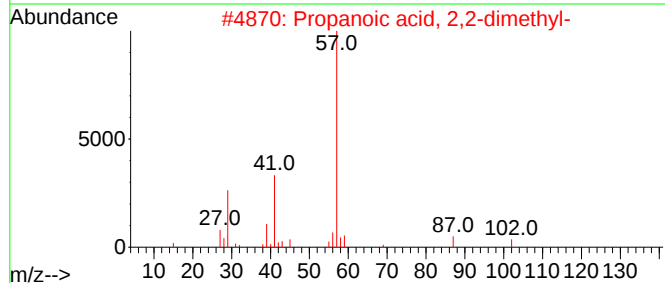
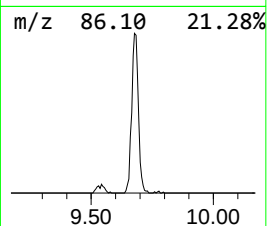
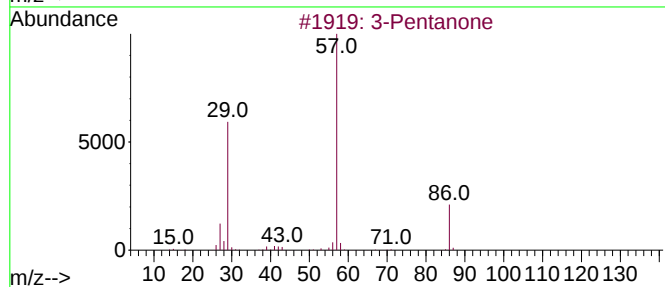
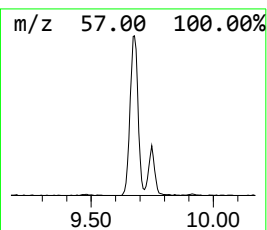
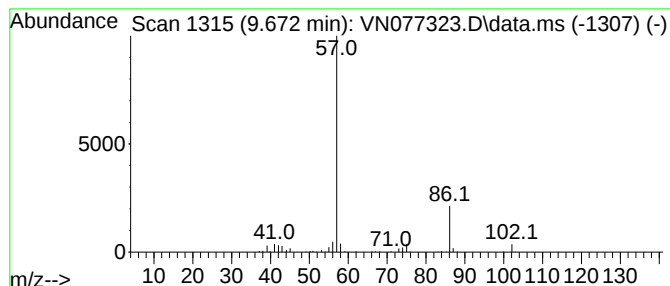
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N040523W.M
Quant Title : SW846 8260

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

Peak Number 1 3-Pentanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.672	8.18 ug/l	391809	1,4-Difluorobenzene	9.107

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone	86	C5H10O	000096-22-0	64
2			Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	32
3			Isobutyl ether	130	C8H18O	000628-55-7	12
4			Ethyl-1-propenyl ether	86	C5H10O	000928-55-2	9
5			Sulfurous acid, dibutyl ester	194	C8H18O3S	000626-85-7	9



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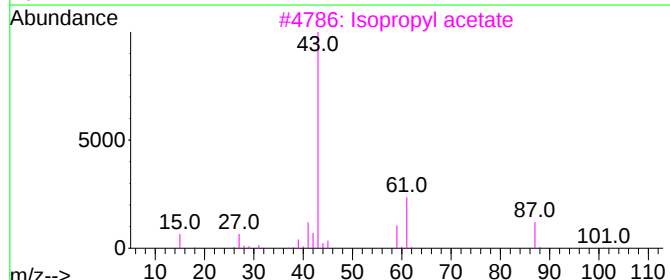
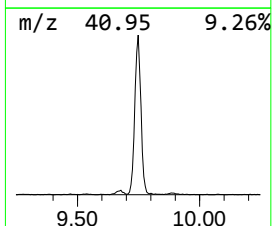
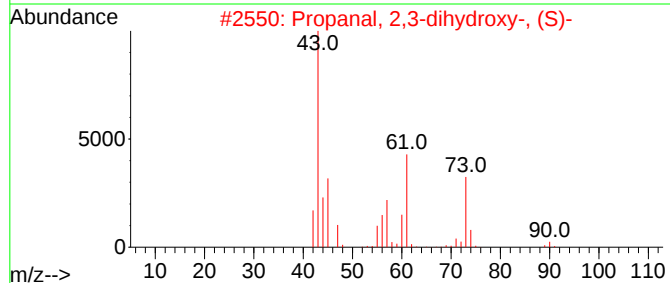
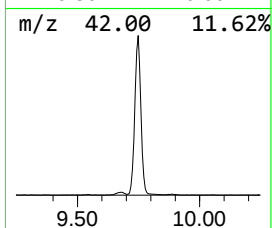
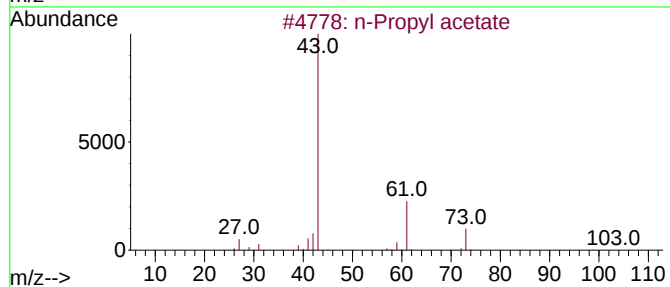
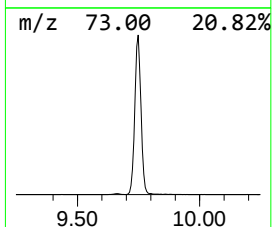
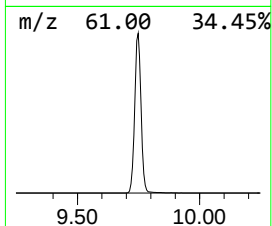
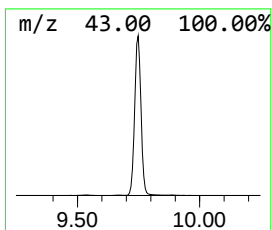
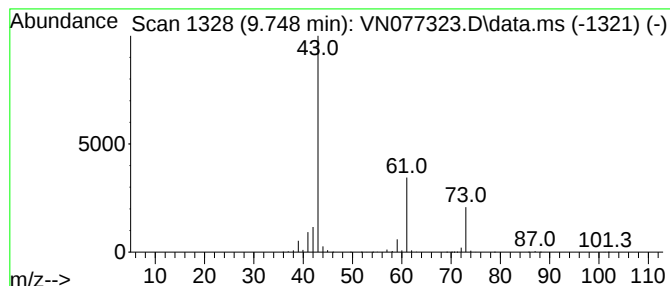
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Quant Title : SW846 8260

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

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.748	145.55 ug/l	6974590	1,4-Difluorobenzene	9.107

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Propyl acetate			102	C5H10O2	000109-60-4	83
2	Propanal, 2,3-dihydroxy-, (S)-			90	C3H6O3	000497-09-6	38
3	Isopropyl acetate			102	C5H10O2	000108-21-4	28
4	Acetamide, N-acetyl-N-methyl-			115	C5H9NO2	001113-68-4	9
5	1-Butanamine			73	C4H11N	000109-73-9	5



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ALS Vial : 9 Sample Multiplier: 1

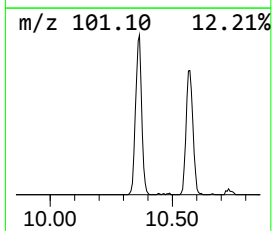
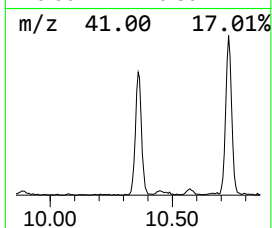
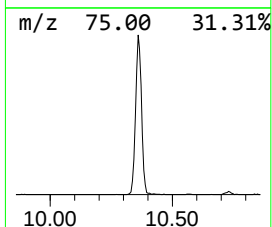
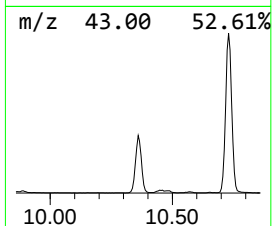
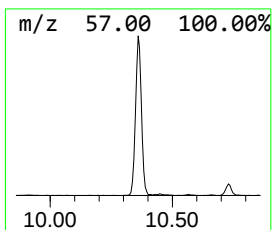
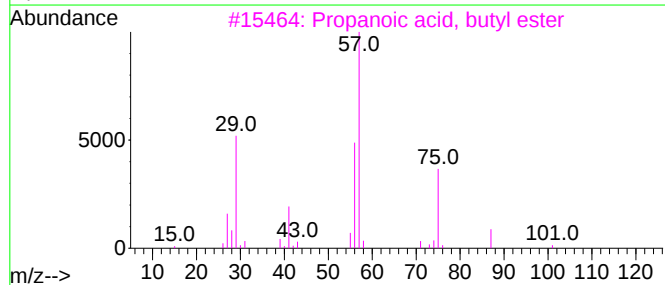
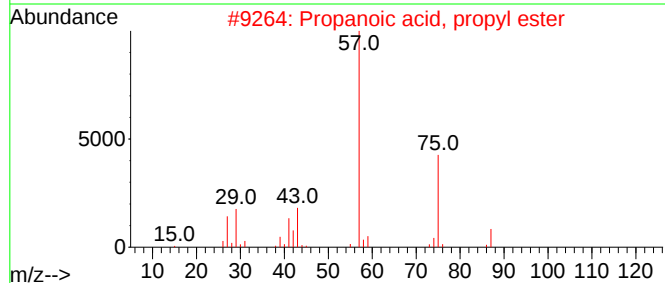
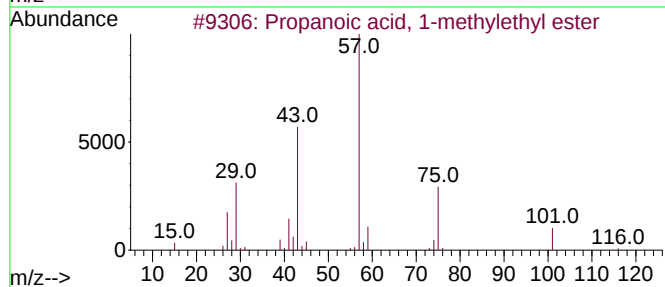
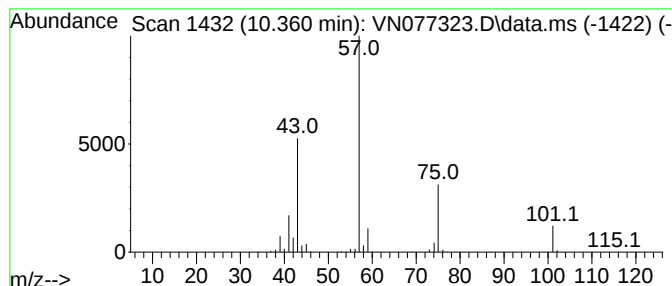
Instrument :
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ClientSampleId :
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Quant Title : SW846 8260

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.	
10.360	31.47 ug/l	1507950	1,4-Difluorobenzene	9.107	
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	25
4	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	14
5	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	9



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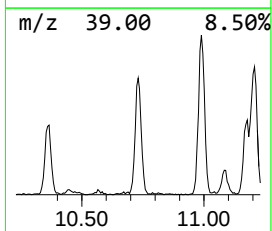
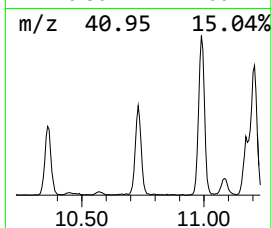
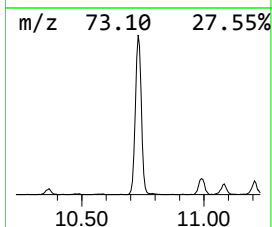
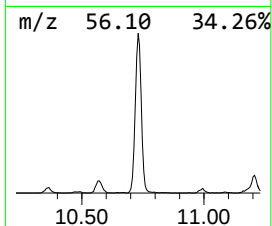
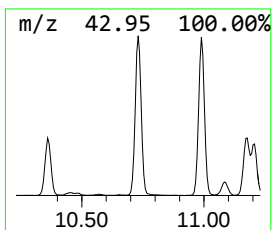
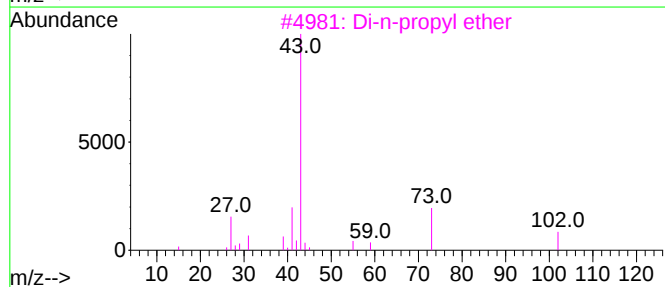
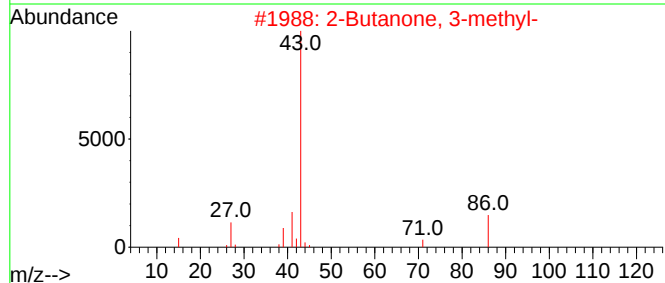
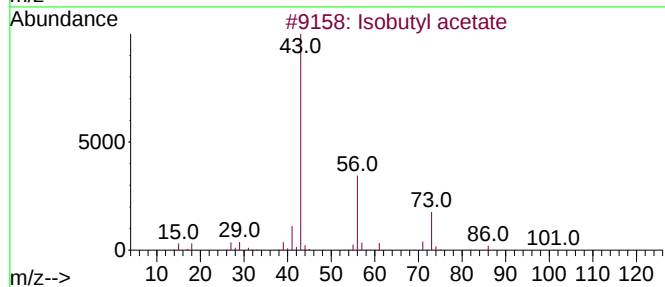
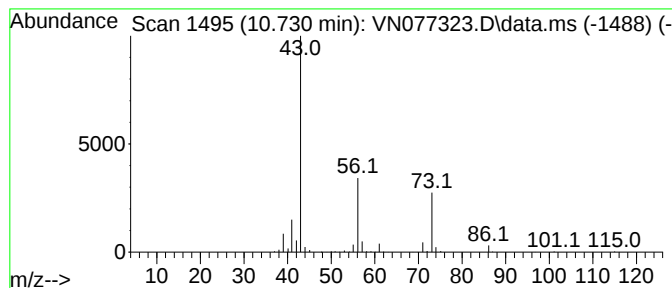
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Peak Number 4 Isobutyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.730	31.52 ug/l	1866090	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutyl acetate	116	C6H12O2	000110-19-0	83
2			2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	22
3			Di-n-propyl ether	102	C6H14O	000111-43-3	17
4			2-Pentanone	86	C5H10O	000107-87-9	9
5			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9



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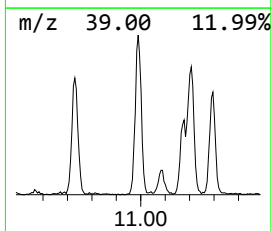
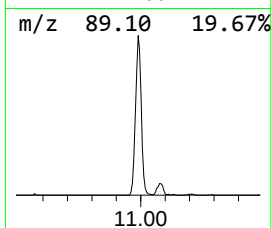
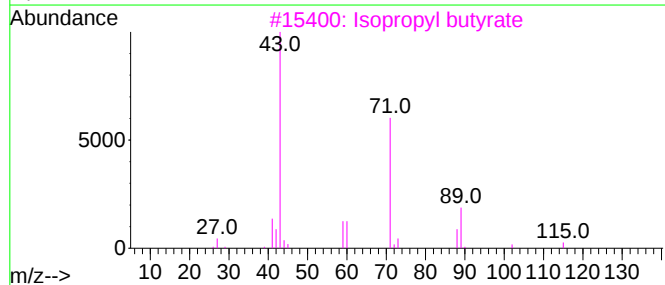
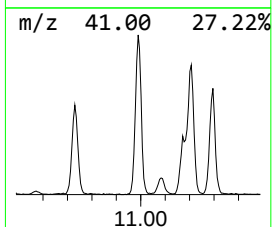
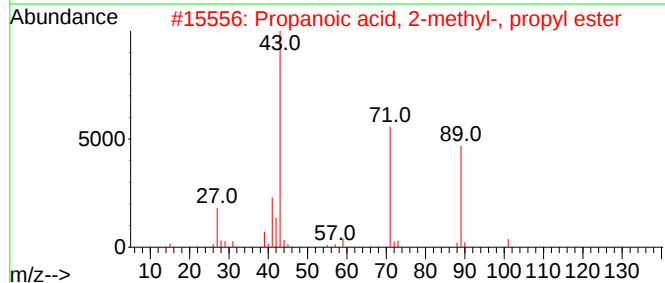
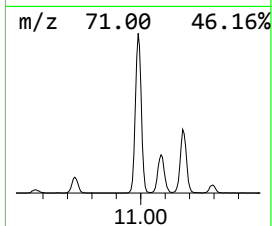
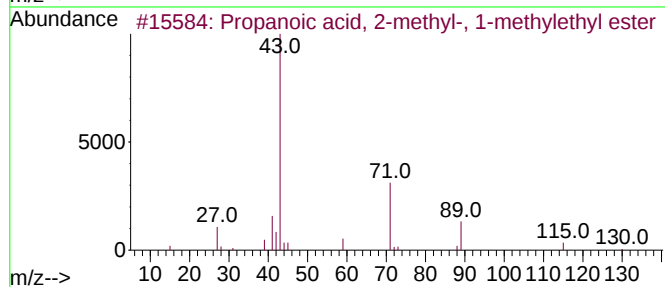
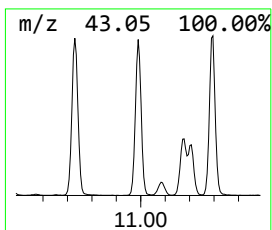
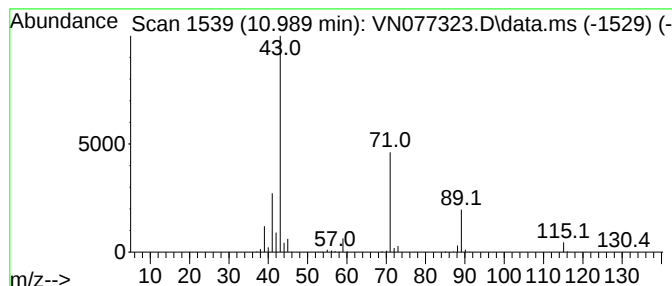
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.989	34.65 ug/l	2051600	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	91
2			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	64
4			Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	50
5			Propanoic acid, 2-methyl-, 2-met...	172	C10H20O2	084254-82-0	40



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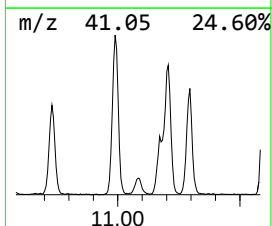
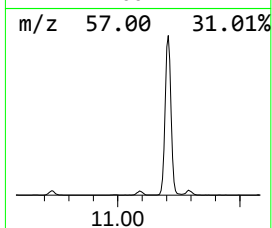
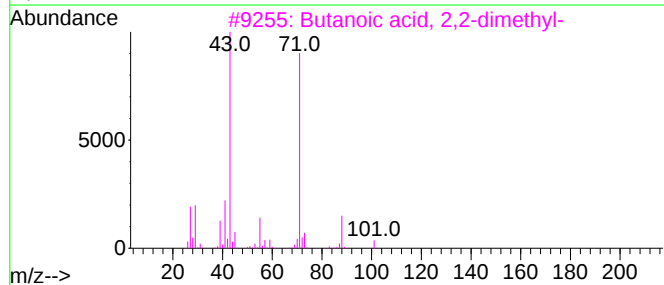
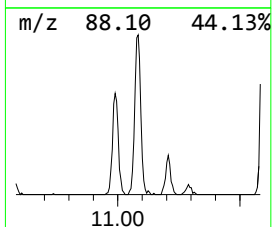
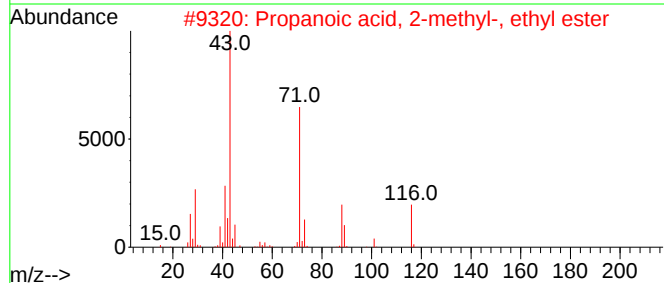
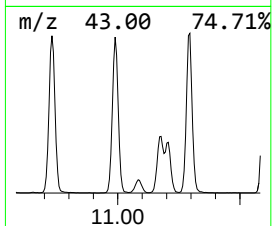
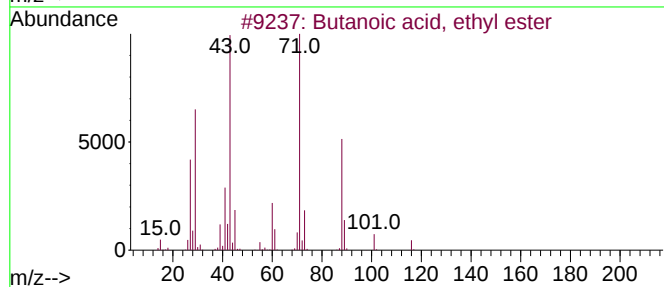
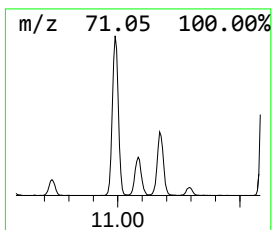
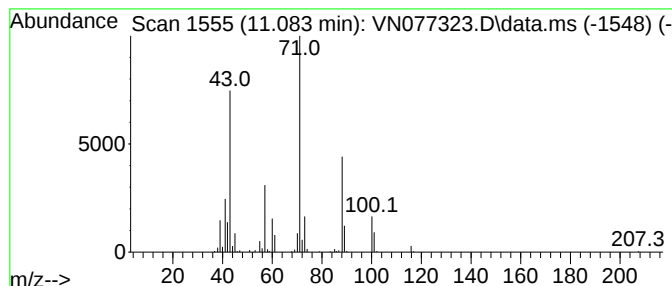
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Quant Title : SW846 8260

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

Peak Number 6 Butanoic acid, ethyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.083	7.41 ug/l	438917	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	90
2			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	70
3			Butanoic acid, 2,2-dimethyl-	116	C6H12O2	000595-37-9	53
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	53
5			3-Mercaptohexyl butanoate	204	C10H20O2S	136954-21-7	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041323\
Data File : VN077323.D
Acq On : 13 Apr 2023 12:58
Operator : JC\MD
Sample : 02292-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
IDW-SO-VB3-041123

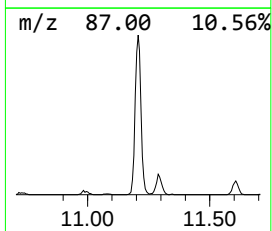
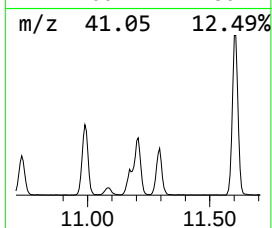
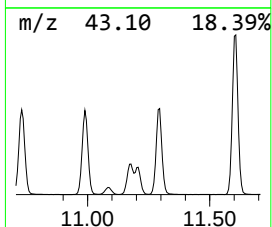
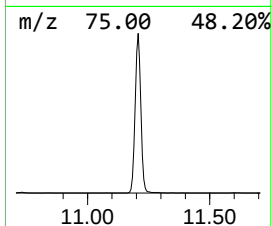
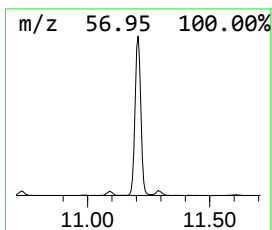
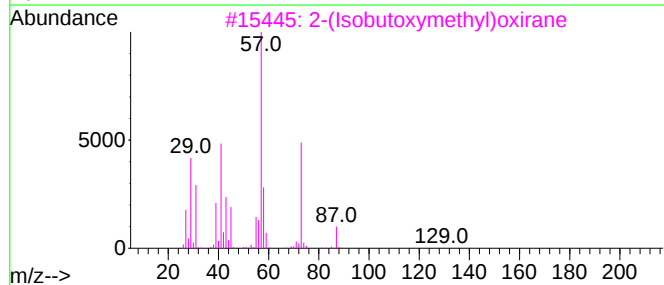
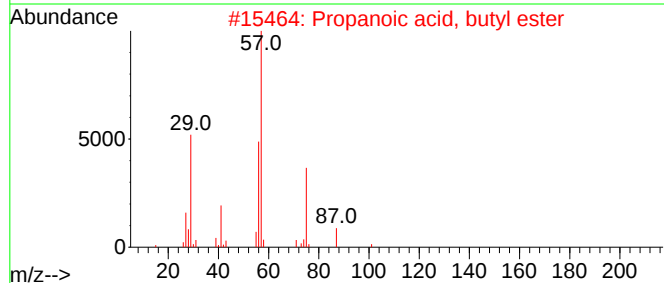
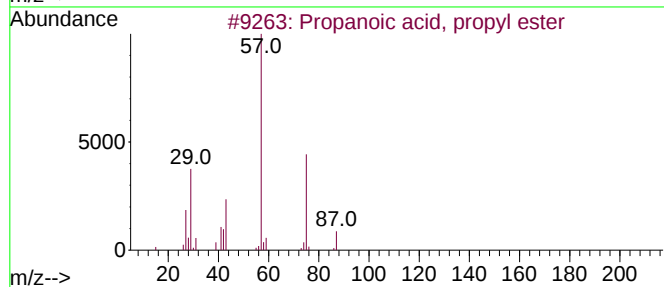
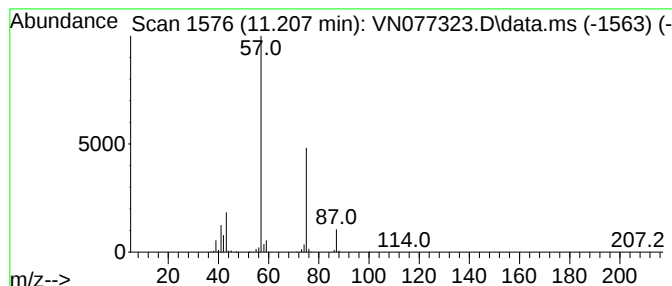
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Quant Title : SW846 8260

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.
11.207	66.32 ug/l	3926710	Chlorobenzene-d5	11.871

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	8
5			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041323\
Data File : VN077323.D
Acq On : 13 Apr 2023 12:58
Operator : JC\MD
Sample : 02292-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
IDW-SO-VB3-041123

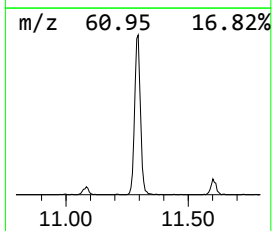
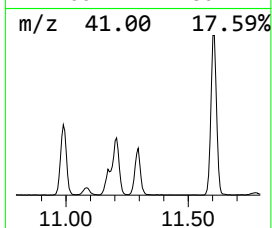
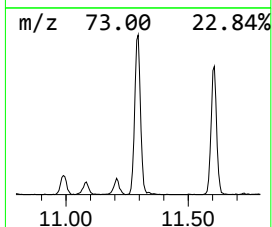
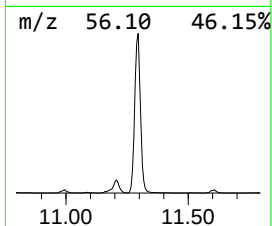
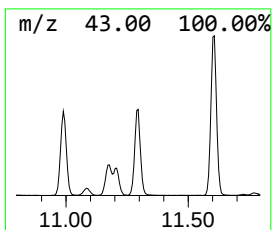
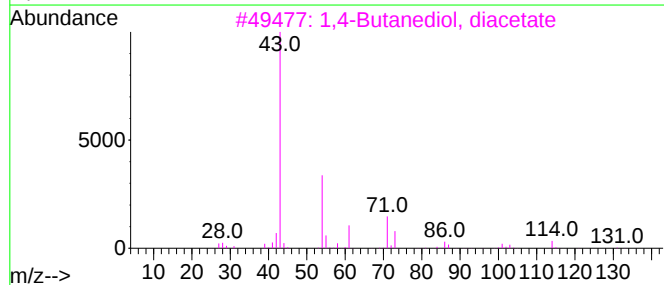
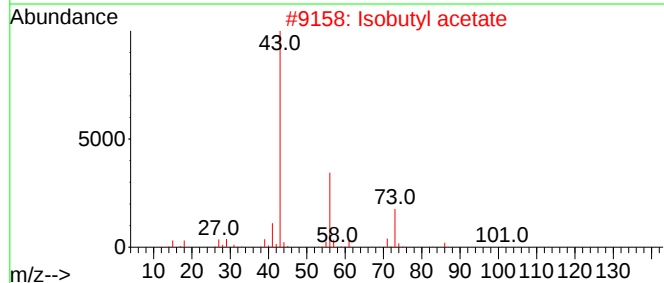
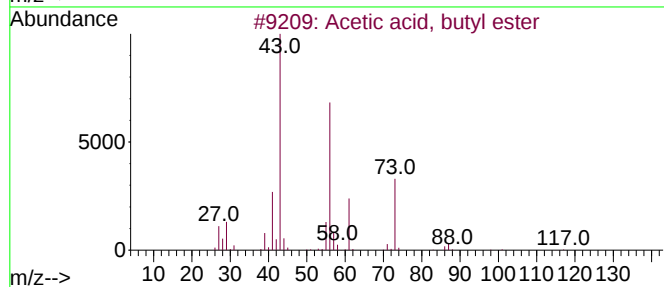
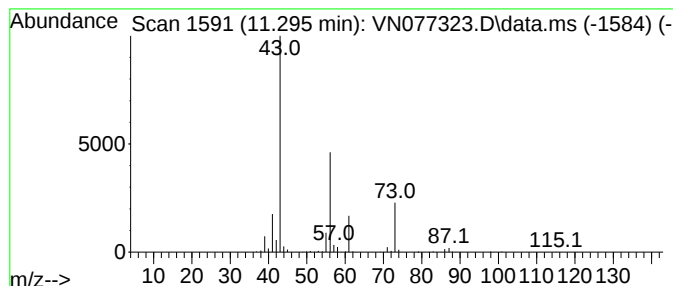
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Quant Title : SW846 8260

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.
11.295	34.76 ug/l	2058350	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	72
2			Isobutyl acetate	116	C6H12O2	000110-19-0	39
3			1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	12
4			Isobutylamine	73	C4H11N	000078-81-9	9
5			Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041323\
Data File : VN077323.D
Acq On : 13 Apr 2023 12:58
Operator : JC\MD
Sample : 02292-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
IDW-SO-VB3-041123

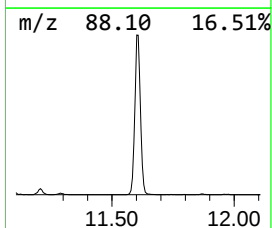
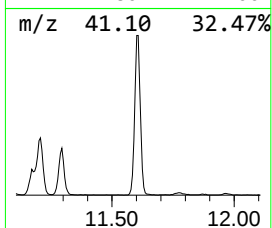
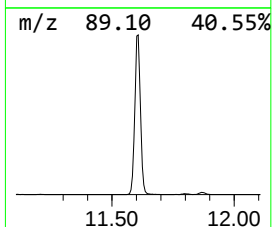
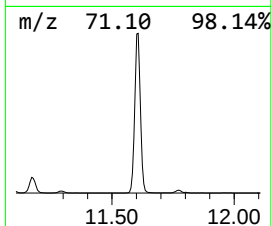
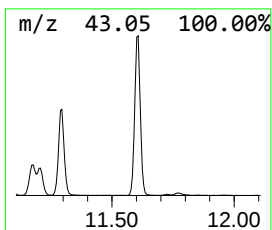
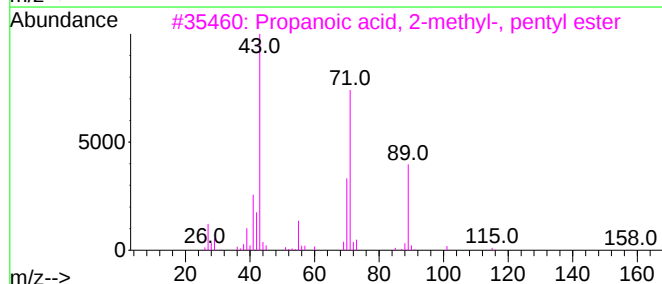
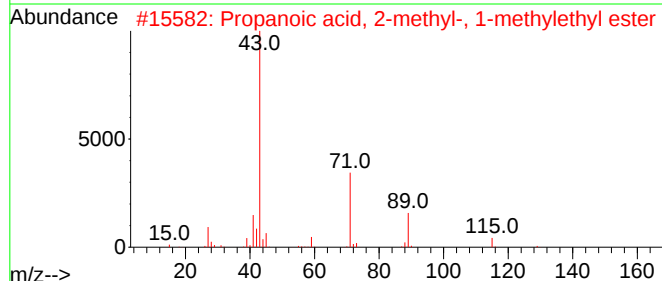
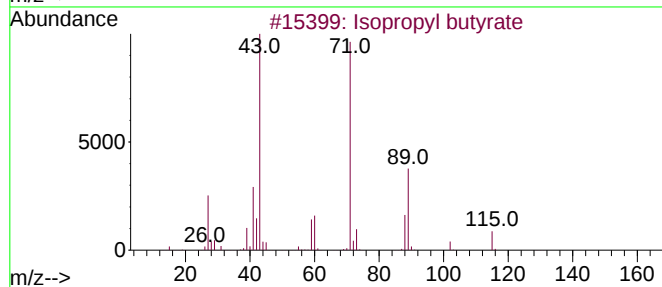
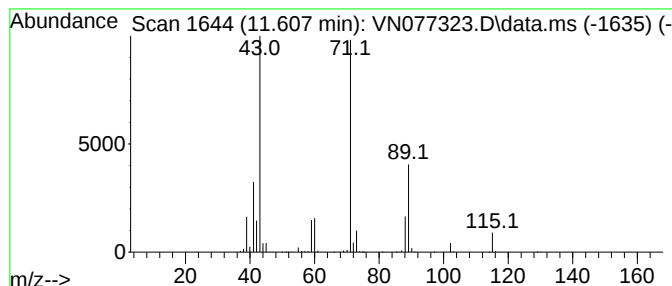
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Quant Title : SW846 8260

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.
11.607	101.08 ug/l	5984760	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl butyrate	130	C7H14O2	000638-11-9	91
2			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	78
3			Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64
4			Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	64
5			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041323\
Data File : VN077323.D
Acq On : 13 Apr 2023 12:58
Operator : JC\MD
Sample : 02292-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
IDW-SO-VB3-041123

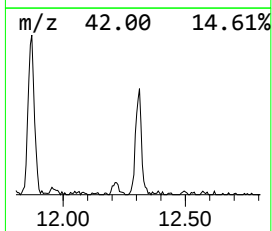
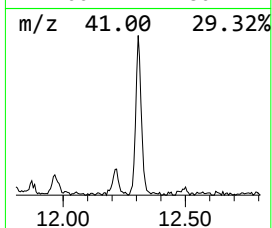
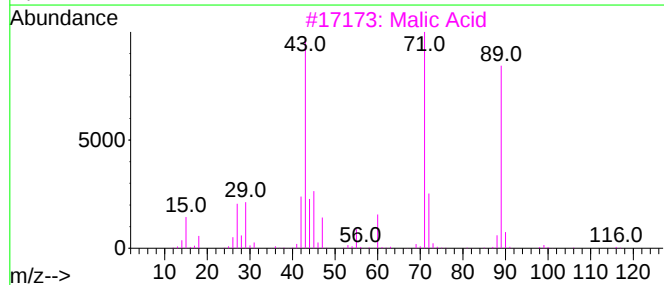
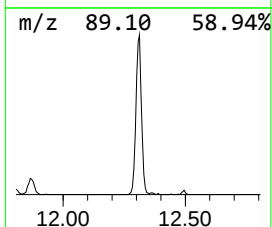
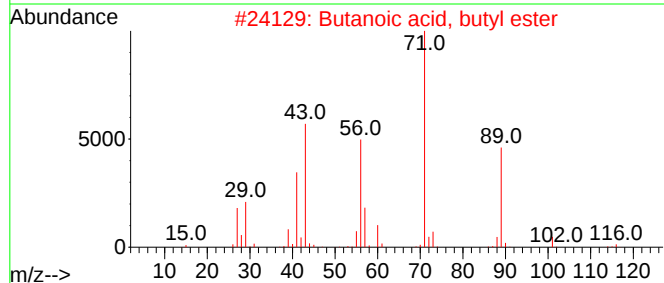
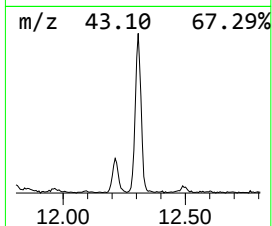
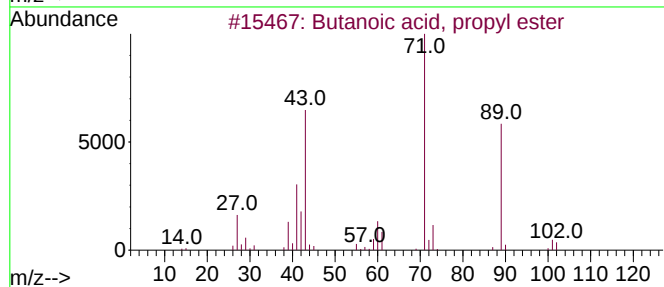
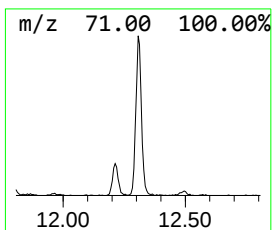
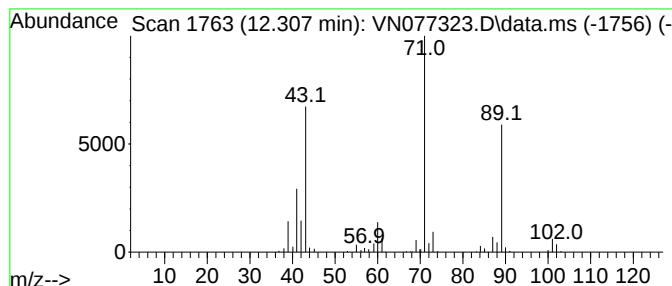
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Quant Title : SW846 8260

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

Peak Number 10 Butanoic acid, propyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.307	9.13 ug/l	540396	Chlorobenzene-d5	11.871

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			Malic Acid	134	C4H6O5	006915-15-7	64
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	50
5			Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN041323\
Data File : VN077323.D
Acq On : 13 Apr 2023 12:58
Operator : JC\MD
Sample : 02292-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
IDW-SO-VB3-041123

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N040523W.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	9.748	145.5	ug/l	6974590	2	9.107	2396000	50.0
Propanoic acid,...	10.360	31.5	ug/l	1507950	2	9.107	2396000	50.0
Isobutyl acetate	10.730	31.5	ug/l	1866090	3	11.871	2960550	50.0
Propanoic acid,...	10.989	34.6	ug/l	2051600	3	11.871	2960550	50.0
Butanoic acid, ...	11.083	7.4	ug/l	438917	3	11.871	2960550	50.0
Propanoic acid,...	11.207	66.3	ug/l	3926710	3	11.871	2960550	50.0
Acetic acid, bu...	11.295	34.8	ug/l	2058350	3	11.871	2960550	50.0
Isopropyl butyrate	11.607	101.1	ug/l	5984760	3	11.871	2960550	50.0
Butanoic acid, ...	12.307	9.1	ug/l	540396	3	11.871	2960550	50.0