

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
 Data File : VN078031.D
 Acq On : 02 Jun 2023 14:57
 Operator : JC\MD
 Sample : 03001-05
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TP17-0A

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\82N051523W.M
 Title : SW846 8260

Signal : TIC: VN078031.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.671	117	122	128	rVB2	33726	59706	1.19%	0.189%
2	2.824	143	148	155	rVB3	27312	60688	1.21%	0.193%
3	4.447	414	424	436	rBV	33457	101908	2.03%	0.323%
4	5.289	555	567	577	rBV3	31919	101834	2.03%	0.323%
5	6.471	758	768	783	rBV3	36130	117683	2.34%	0.373%
6	7.571	949	955	968	rVB3	46846	123636	2.46%	0.392%
7	8.177	1047	1058	1062	rBV	339127	799962	15.93%	2.539%
8	8.235	1062	1068	1081	rVB	587027	1313101	26.15%	4.167%
9	8.588	1118	1128	1137	rBV3	371815	1044446	20.80%	3.315%
10	8.700	1137	1147	1158	rVV2	323714	880639	17.53%	2.795%
11	9.112	1208	1217	1229	rBV	869717	1799910	35.84%	5.712%
12	9.677	1305	1313	1318	rBV	133284	288122	5.74%	0.914%
13	9.753	1318	1326	1343	rVV	2707693	5022284	100.00%	15.939%
14	10.365	1421	1430	1441	rBV	613988	1044490	20.80%	3.315%
15	10.576	1456	1466	1476	rBV	1346980	2518888	50.15%	7.994%
16	10.735	1485	1493	1507	rVB	620728	1059176	21.09%	3.361%
17	10.994	1530	1537	1546	rBV	803279	1321938	26.32%	4.195%
18	11.088	1546	1553	1561	rVV3	158559	293405	5.84%	0.931%
19	11.212	1561	1574	1582	rVV2	1226179	2571237	51.20%	8.160%
20	11.294	1582	1588	1599	rVB	734608	1215478	24.20%	3.858%
21	11.606	1633	1641	1654	rBV	2298915	3680978	73.29%	11.682%
22	11.771	1665	1669	1678	rVB3	36902	68880	1.37%	0.219%
23	11.871	1678	1686	1698	rVV	1172617	2164602	43.10%	6.870%
24	11.971	1698	1703	1711	rVB2	59571	101614	2.02%	0.322%
25	12.218	1737	1745	1753	rBV2	28171	52286	1.04%	0.166%
26	12.312	1753	1761	1771	rBV	184116	299214	5.96%	0.950%
27	12.853	1847	1853	1863	rVB	894281	1593098	31.72%	5.056%
28	13.800	2006	2014	2024	rBV	870879	1504894	29.96%	4.776%
29	14.000	2042	2048	2056	rVB	121620	213208	4.25%	0.677%
30	15.647	2320	2328	2336	rBV	46627	91778	1.83%	0.291%

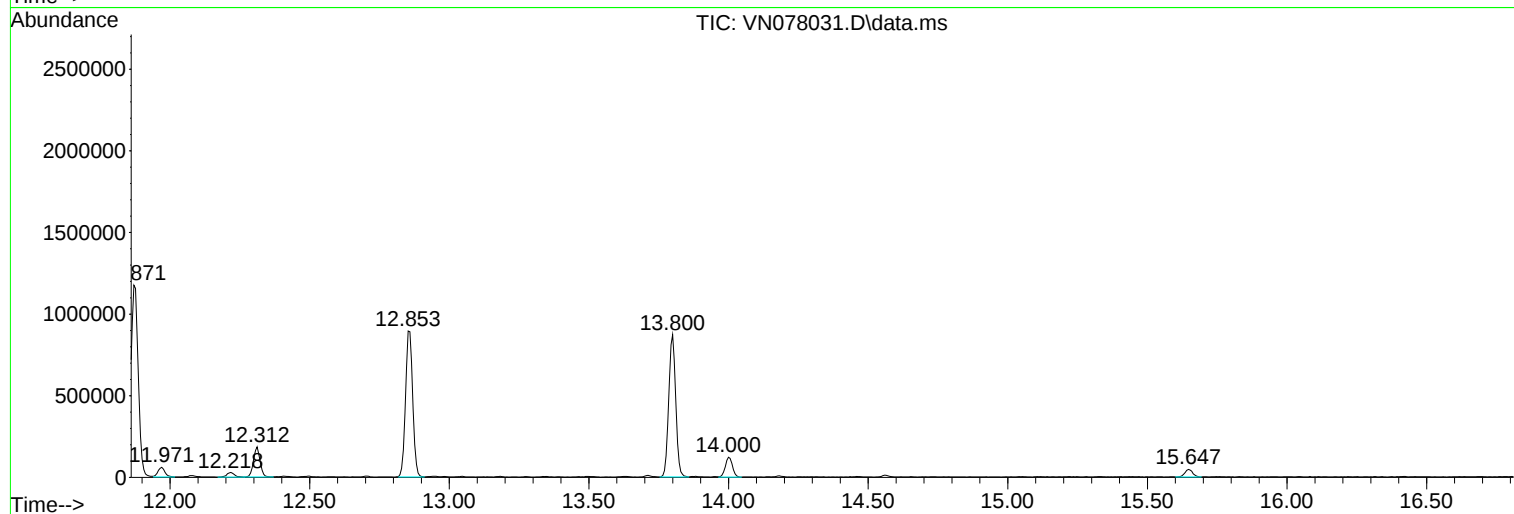
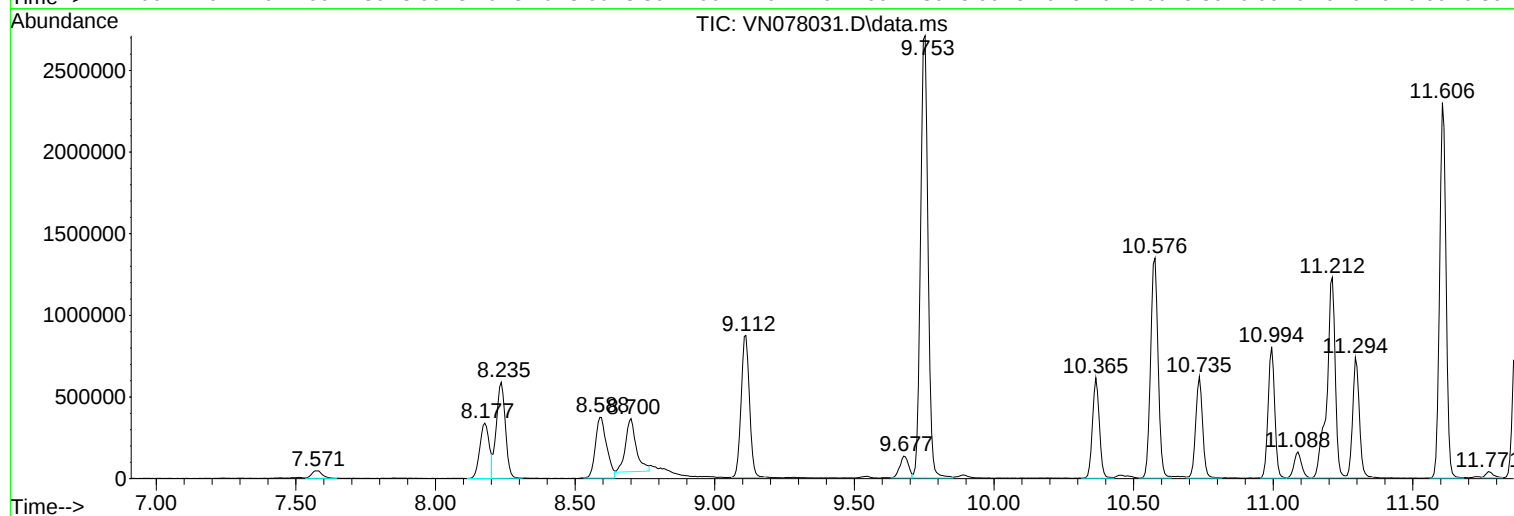
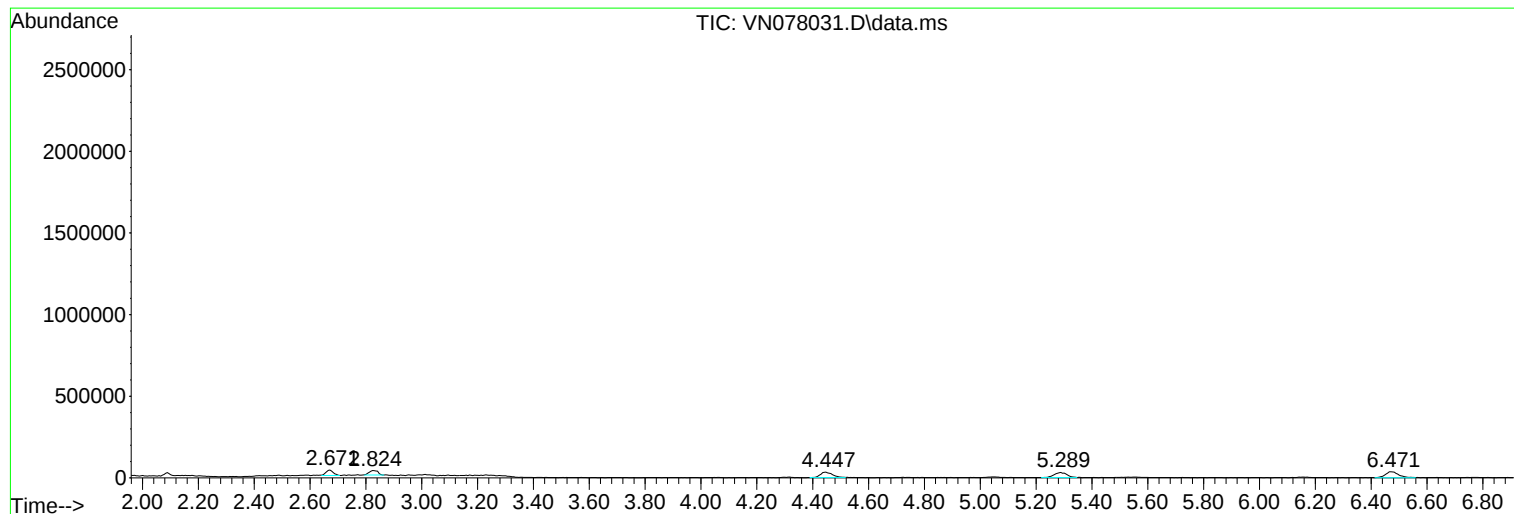
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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



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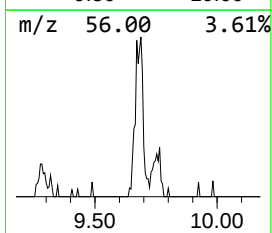
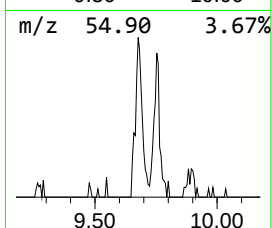
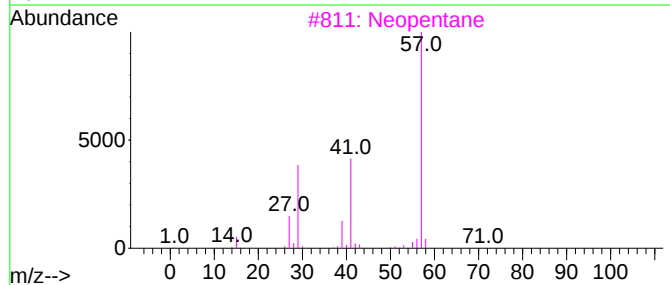
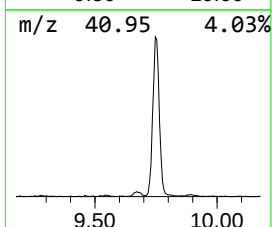
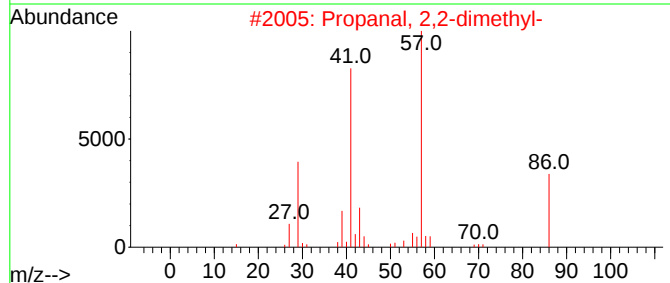
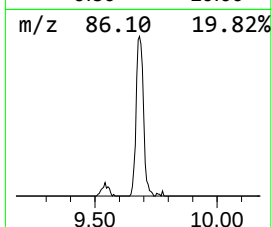
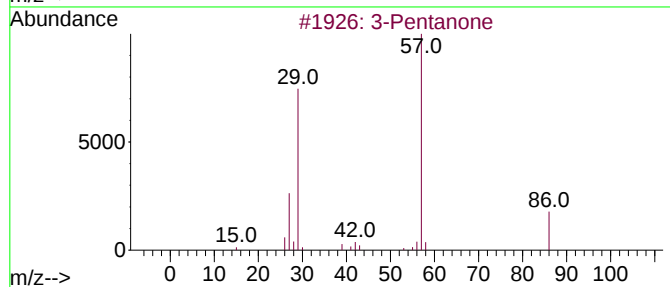
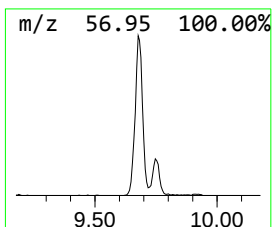
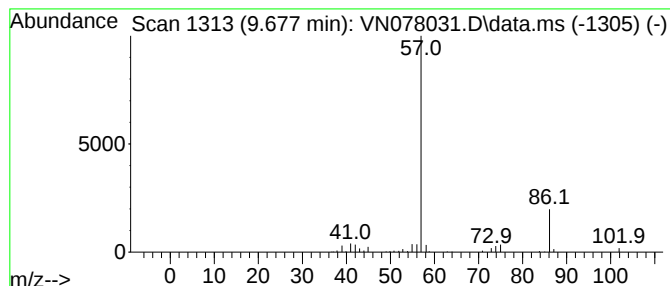
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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

Peak Number 1 3-Pentanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.677	8.00 ug/l	288122	1,4-Difluorobenzene	9.112

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone	86	C5H10O	000096-22-0	64
2			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	40
3			Neopentane	72	C5H12	000463-82-1	23
4			Oxalic acid, ethyl isobutyl ester	174	C8H14O4	1000309-36-7	23
5			Ethyl-1-propenyl ether	86	C5H10O	000928-55-2	9



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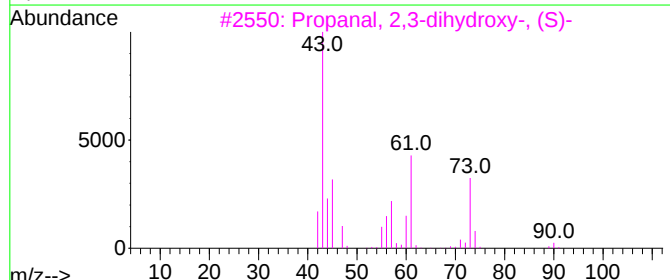
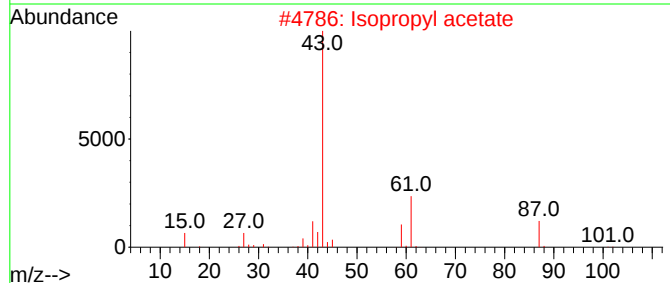
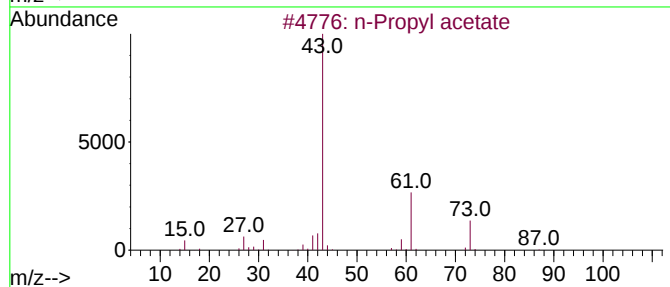
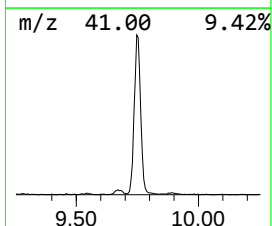
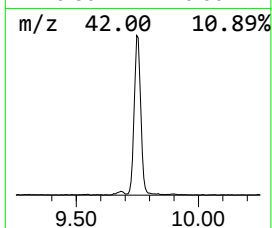
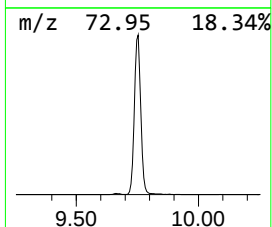
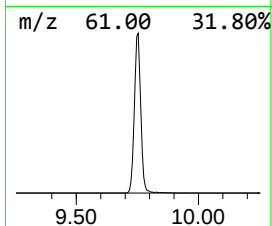
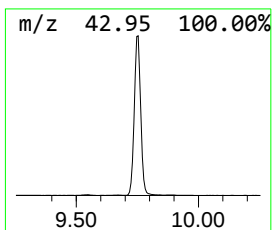
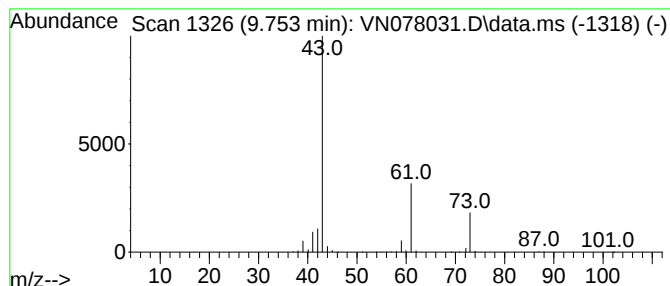
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Quant Title : SW846 8260

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.
9.753	139.51 ug/l	5022280	1,4-Difluorobenzene	9.112

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	38
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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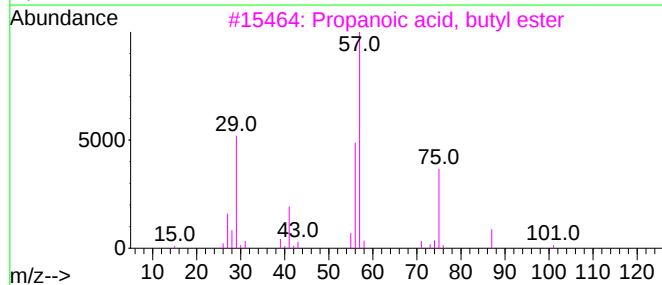
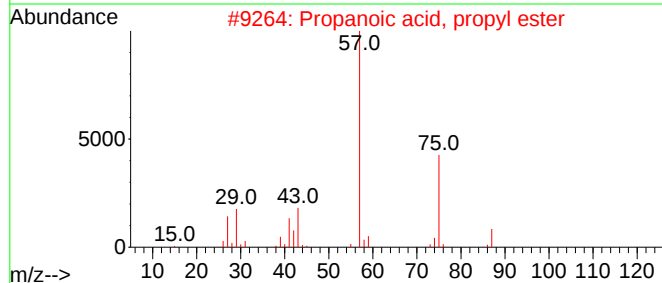
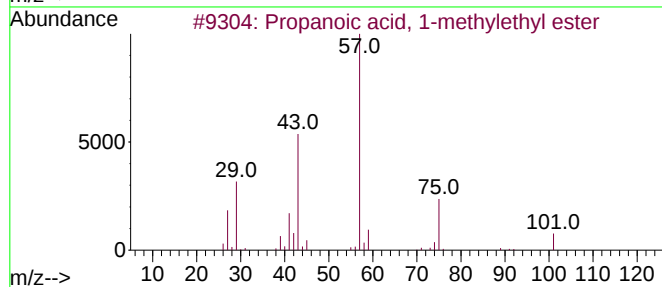
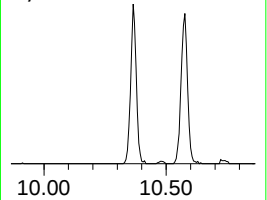
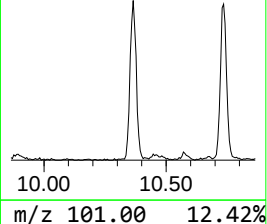
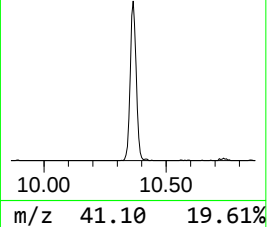
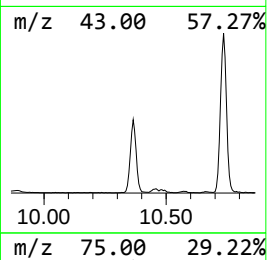
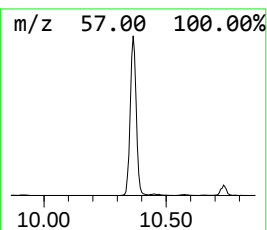
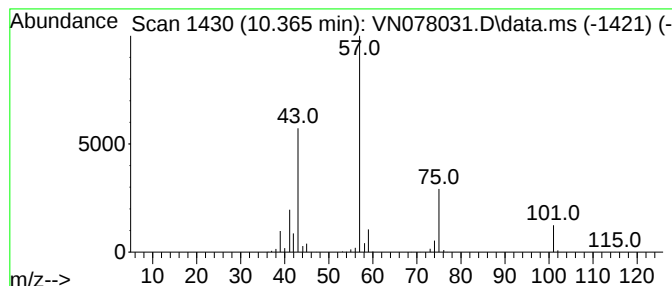
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.365	29.02 ug/l	1044490	1,4-Difluorobenzene	9.112

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			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10



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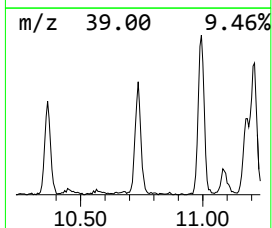
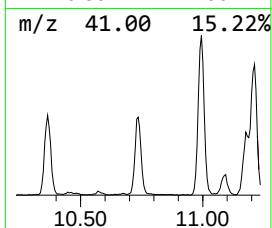
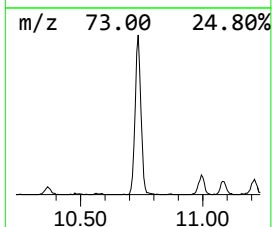
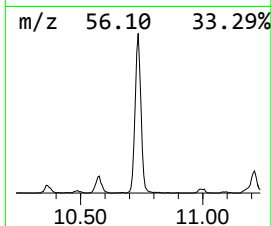
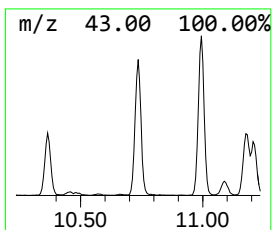
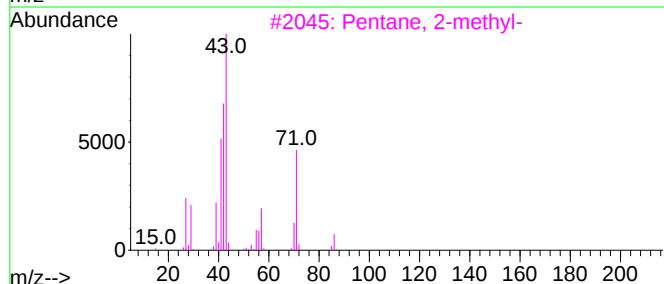
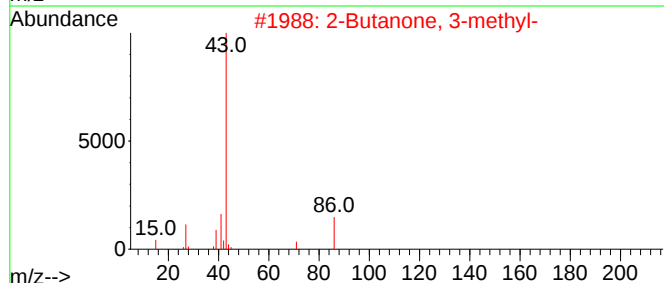
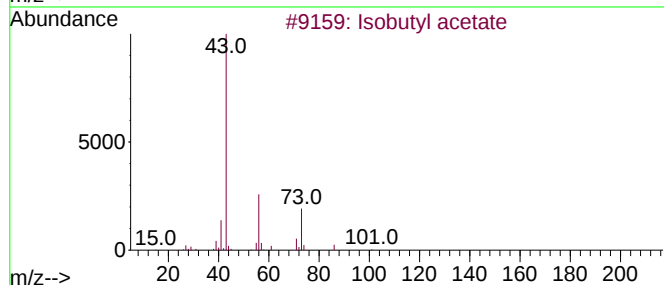
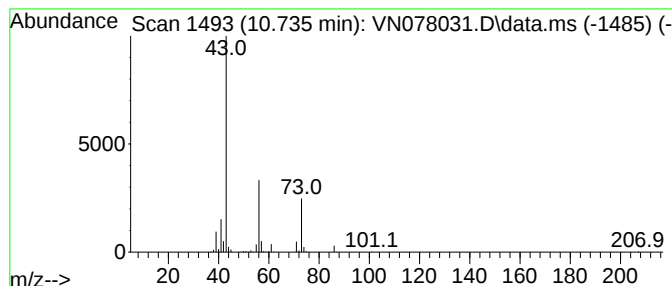
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Peak Number 4 Isobutyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.735	24.47 ug/l	1059180	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			Pentane, 2-methyl-	86	C6H14	000107-83-5	9
4			3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	9
5			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9



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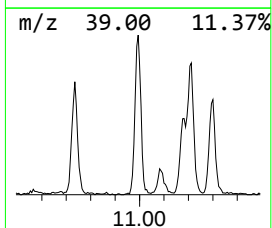
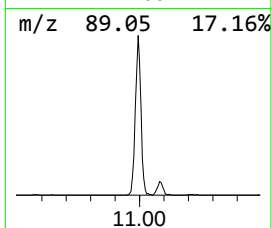
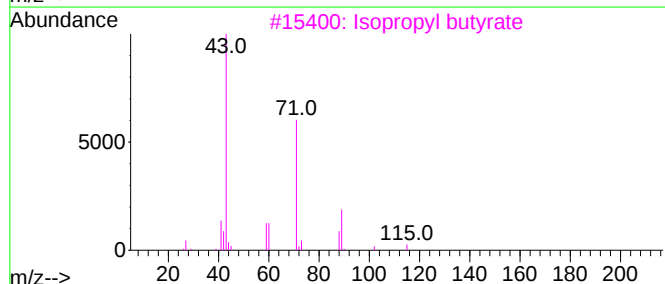
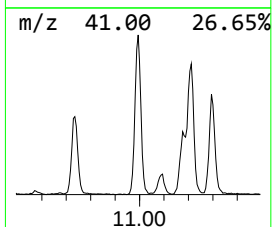
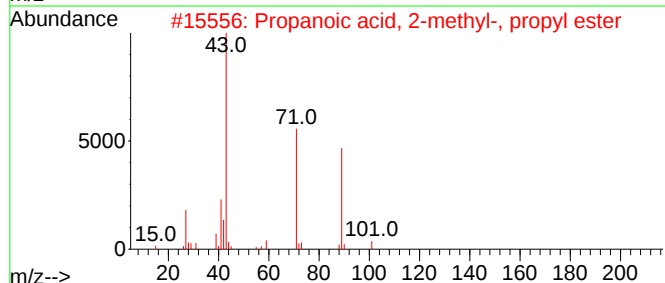
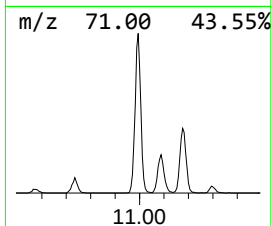
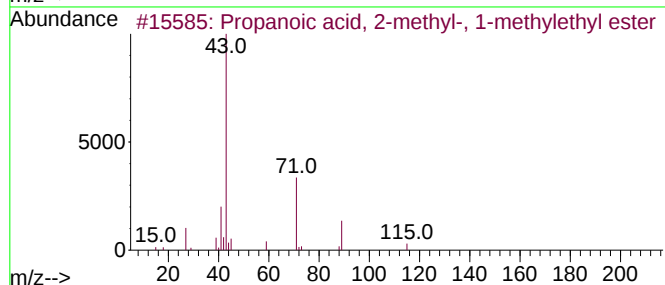
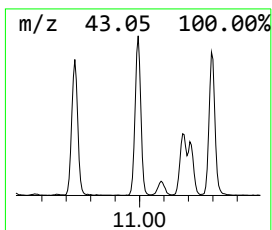
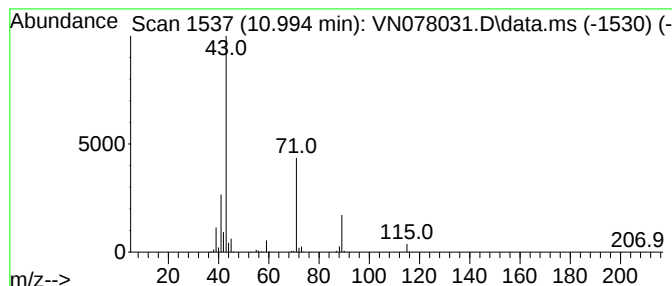
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Quant Title : SW846 8260

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

Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.994	30.54 ug/l	1321940	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	83
2			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	78
3			Isopropyl butyrate	130	C7H14O2	000638-11-9	56
4			2,3-Hexanedione	114	C6H10O2	003848-24-6	53
5			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42



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TP17-0A

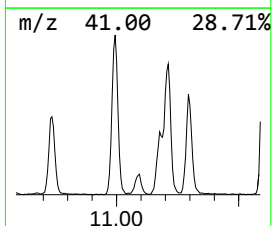
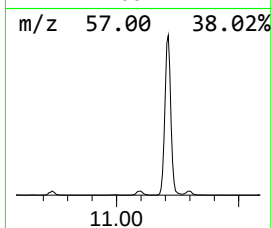
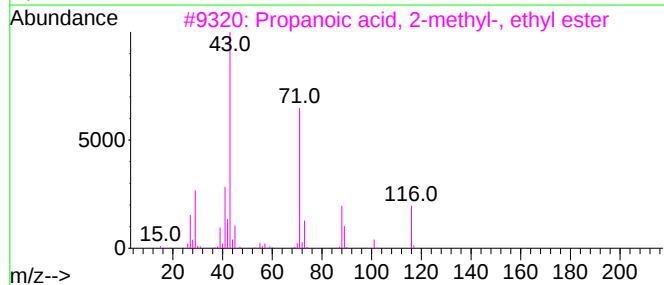
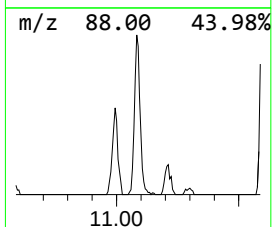
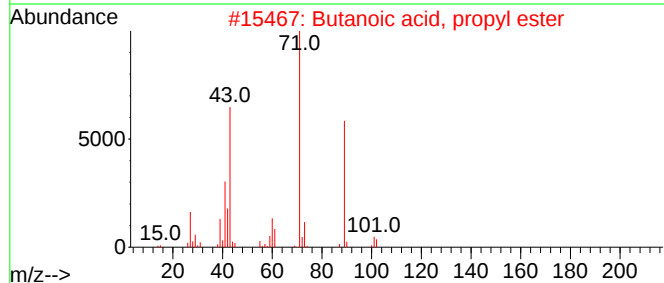
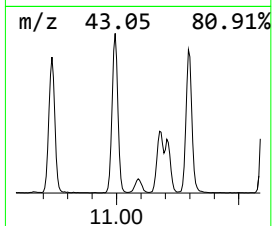
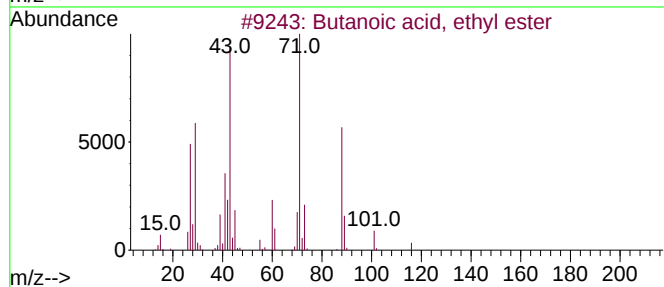
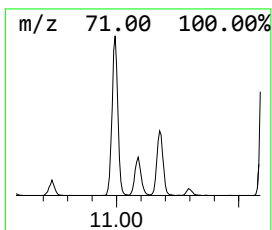
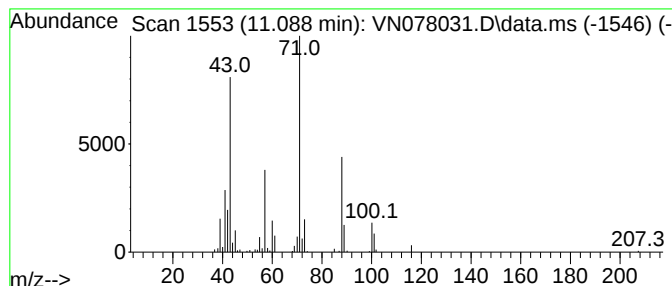
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Quant Title : SW846 8260

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.
11.088	6.78 ug/l	293405	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	89
2			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	53
3			Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	45
4			n-Amyl ether	158	C10H22O	000693-65-2	43
5			Butanoic acid, anhydride	158	C8H14O3	000106-31-0	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078031.D
Acq On : 02 Jun 2023 14:57
Operator : JC\MD
Sample : 03001-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP17-0A

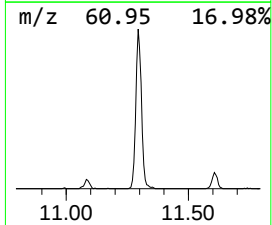
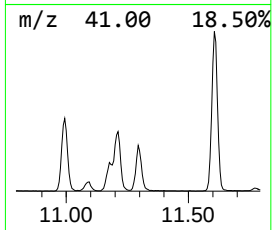
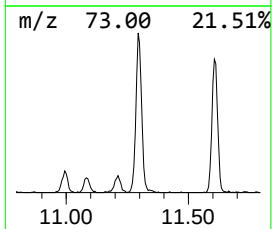
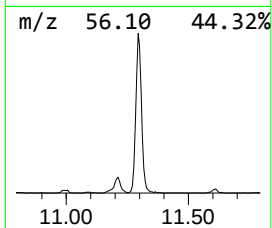
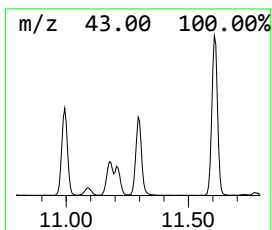
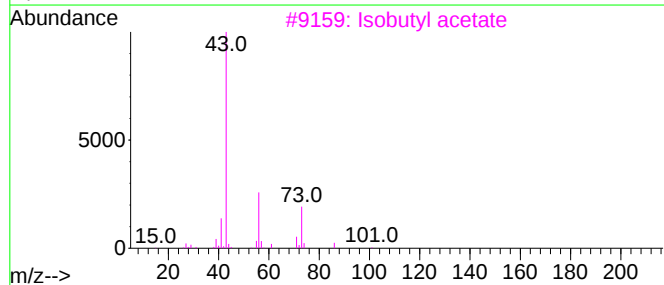
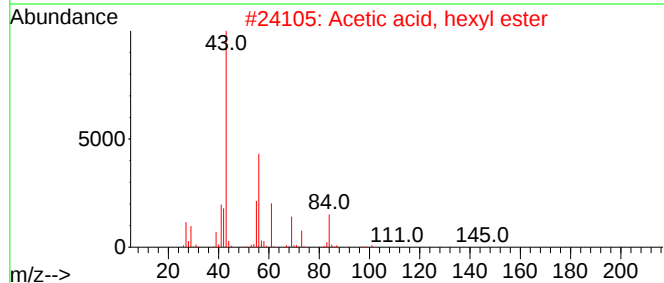
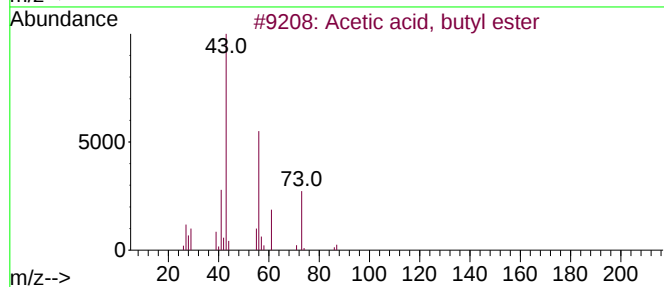
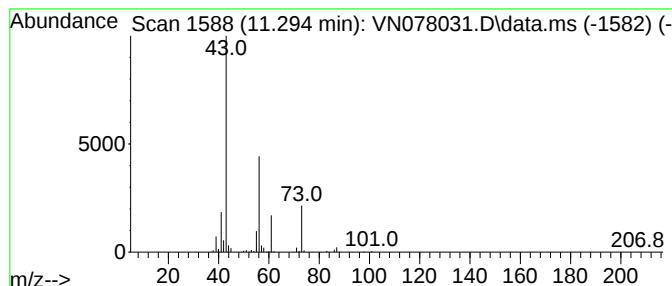
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Quant Title : SW846 8260

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

Peak Number 7 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.294	28.08 ug/l	1215480	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2			Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	36
3			Isobutyl acetate	116	C6H12O2	000110-19-0	28
4			Isobutylamine	73	C4H11N	000078-81-9	9
5			2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078031.D
Acq On : 02 Jun 2023 14:57
Operator : JC\MD
Sample : 03001-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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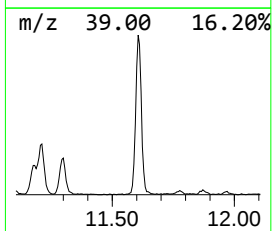
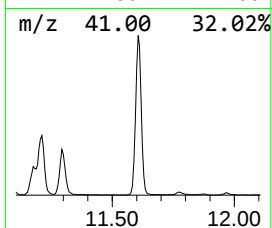
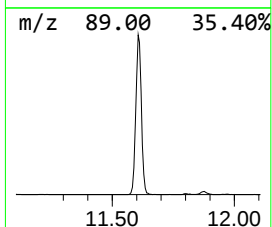
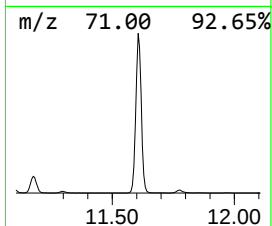
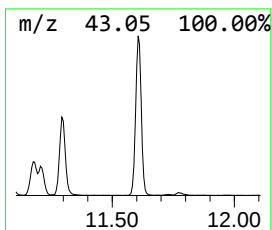
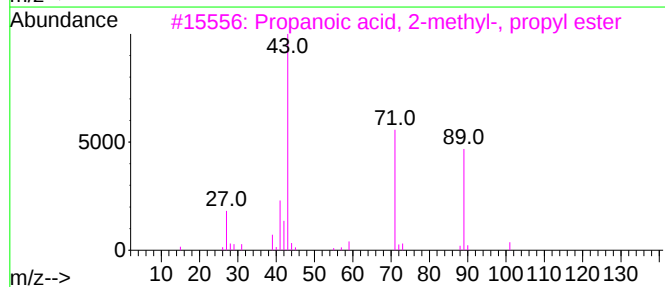
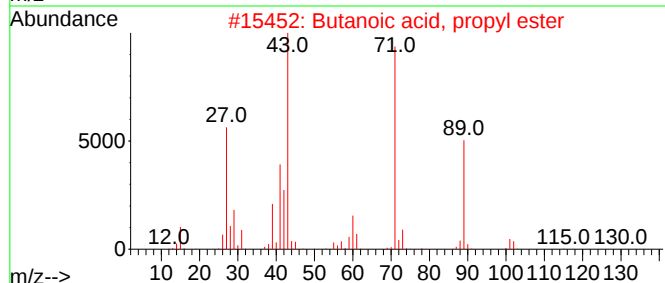
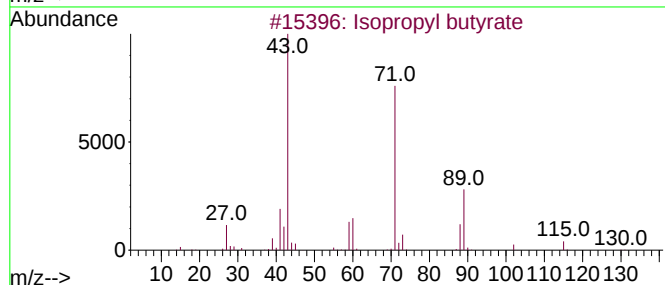
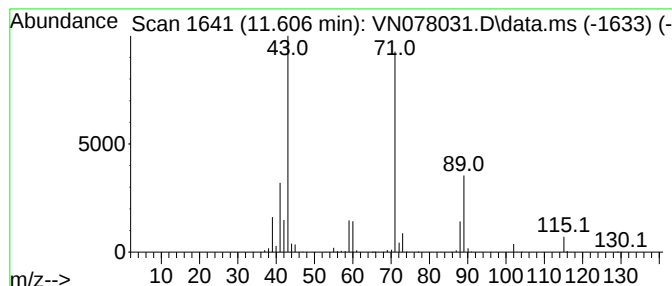
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Quant Title : SW846 8260

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

Peak Number 8 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.606	85.03 ug/l	3680980	Chlorobenzene-d5	11.871

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-, propy...	130	C7H14O2	000644-49-5	72
4			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
5			Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078031.D
Acq On : 02 Jun 2023 14:57
Operator : JC\MD
Sample : 03001-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP17-0A

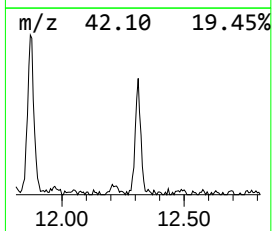
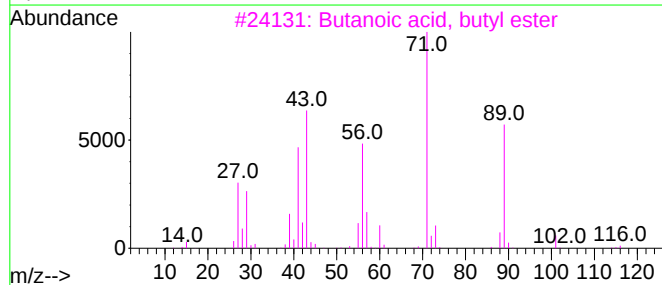
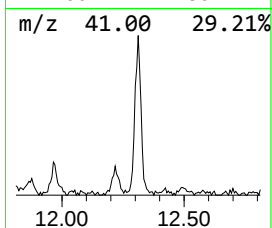
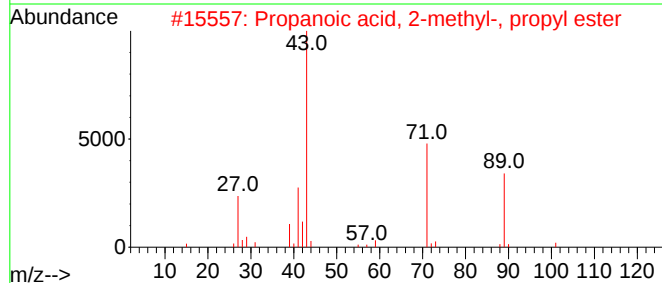
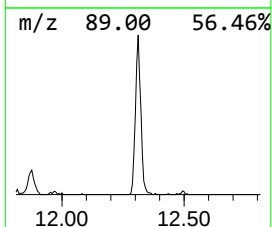
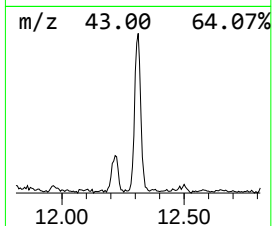
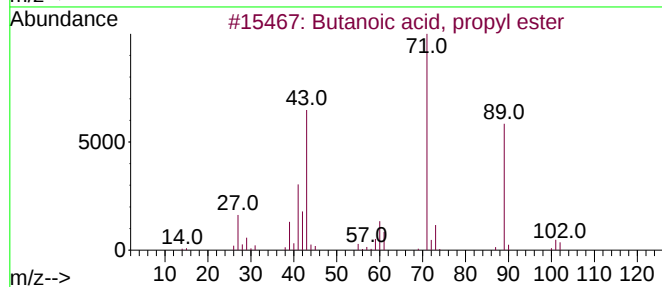
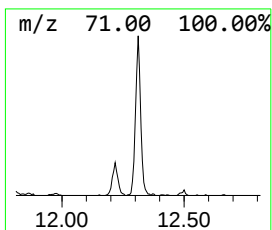
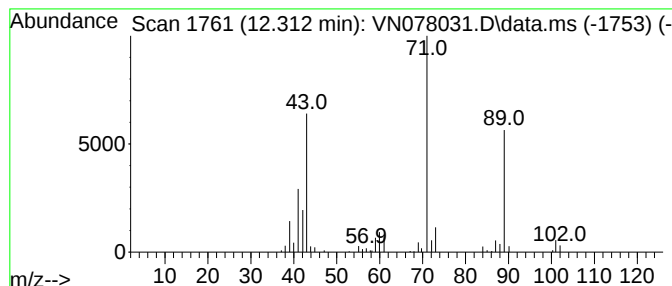
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Quant Title : SW846 8260

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.
12.312	6.91 ug/l	299214	Chlorobenzene-d5	11.871

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	86
2			Propanoic acid, 2-methyl-, propyl ester	130	C7H14O2	000644-49-5	72
3			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	56
4			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	53
5			Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078031.D
Acq On : 02 Jun 2023 14:57
Operator : JC\MD
Sample : 03001-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP17-0A

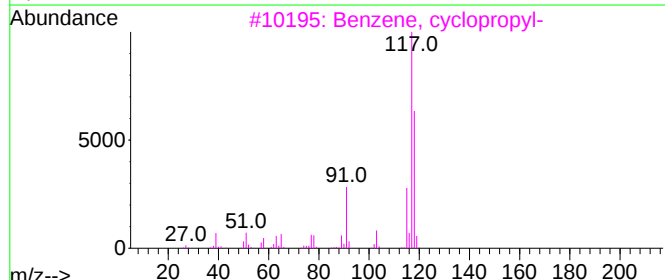
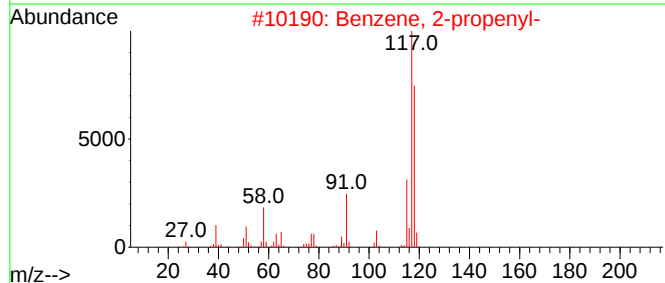
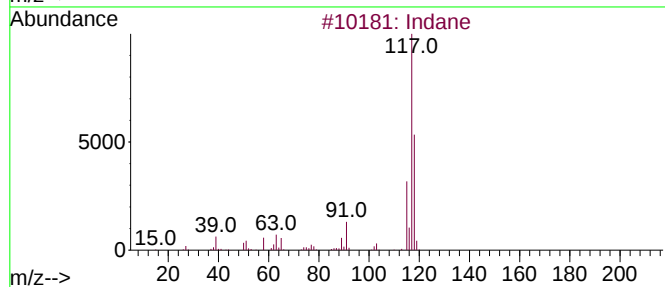
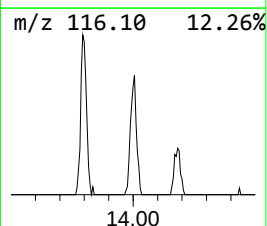
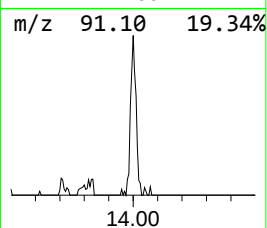
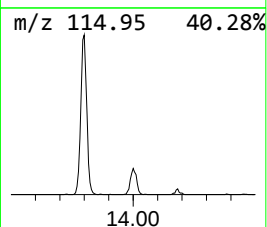
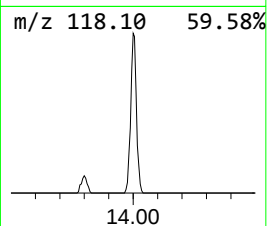
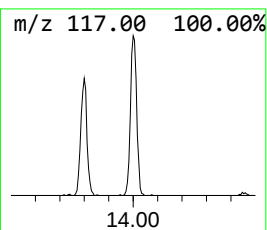
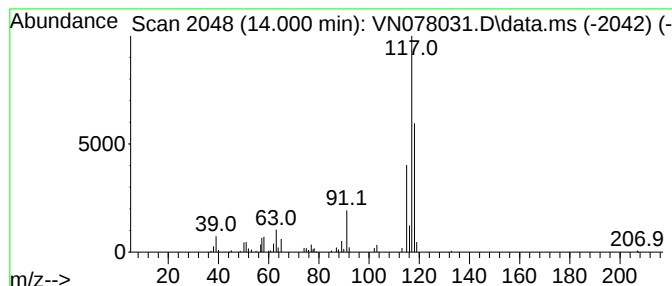
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Quant Title : SW846 8260

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

Peak Number 10 Indane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.000	7.08 ug/l	213208	1,4-Dichlorobenzene-d4	13.800

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	93
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	58
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	58
4			Benzene, 1-propenyl-	118	C9H10	000637-50-3	58
5			trans-Cinnamyl bromide	196	C9H9Br	026146-77-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078031.D
Acq On : 02 Jun 2023 14:57
Operator : JC\MD
Sample : 03001-05
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP17-0A

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.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	9.753	139.5	ug/l	5022280	2	9.112	1799910	50.0
Propanoic acid,...	10.365	29.0	ug/l	1044490	2	9.112	1799910	50.0
Isobutyl acetate	10.735	24.5	ug/l	1059180	3	11.871	2164600	50.0
Propanoic acid,...	10.994	30.5	ug/l	1321940	3	11.871	2164600	50.0
Butanoic acid, ...	11.088	6.8	ug/l	293405	3	11.871	2164600	50.0
Acetic acid, bu...	11.294	28.1	ug/l	1215480	3	11.871	2164600	50.0
Isopropyl butyrate	11.606	85.0	ug/l	3680980	3	11.871	2164600	50.0
Butanoic acid, ...	12.312	6.9	ug/l	299214	3	11.871	2164600	50.0
Indane	14.000	7.1	ug/l	213208	4	13.800	1504890	50.0