

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
 Data File : VN078030.D
 Acq On : 02 Jun 2023 14:33
 Operator : JC\MD
 Sample : 03001-02
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 TP16-0A

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: VN078030.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.089	17	23	28	rBV4	20504	30858	1.12%	0.128%
2	2.671	117	122	127	rBV	39256	60203	2.18%	0.250%
3	2.830	141	149	154	rVB2	32029	75202	2.72%	0.313%
4	4.441	411	423	424	rBV2	37571	62621	2.27%	0.260%
5	5.288	556	567	580	rVB3	35411	107650	3.90%	0.448%
6	6.471	756	768	782	rBV4	15647	47217	1.71%	0.196%
7	7.571	948	955	967	rVB2	40430	99317	3.60%	0.413%
8	8.177	1048	1058	1062	rBV	303179	711428	25.78%	2.959%
9	8.235	1062	1068	1079	rVB	508454	1172873	42.50%	4.879%
10	8.594	1111	1129	1138	rBV4	374481	1314567	47.63%	5.468%
11	8.700	1138	1147	1180	rVB2	315418	1426570	51.69%	5.934%
12	9.112	1208	1217	1230	rVB	767254	1587081	57.50%	6.602%
13	9.676	1305	1313	1319	rBV	125864	276106	10.00%	1.149%
14	9.747	1319	1325	1340	rVV	1473439	2759905	100.00%	11.480%
15	9.888	1344	1349	1358	rVB6	12103	28753	1.04%	0.120%
16	10.365	1422	1430	1440	rBV	529866	916293	33.20%	3.811%
17	10.459	1440	1446	1457	rVB5	18947	46204	1.67%	0.192%
18	10.576	1457	1466	1478	rBV	1191731	2230358	80.81%	9.277%
19	10.735	1487	1493	1500	rVB	109688	185671	6.73%	0.772%
20	10.994	1528	1537	1546	rBV	681555	1135917	41.16%	4.725%
21	11.088	1546	1553	1561	rVB2	121592	229205	8.30%	0.953%
22	11.212	1569	1574	1582	rVB	926200	1634743	59.23%	6.800%
23	11.300	1582	1589	1597	rVB	172874	300127	10.87%	1.248%
24	11.606	1634	1641	1654	rBV	1606955	2577967	93.41%	10.723%
25	11.776	1665	1670	1678	rVB3	32477	61536	2.23%	0.256%
26	11.870	1678	1686	1698	rVV	1050444	1885493	68.32%	7.843%
27	11.970	1698	1703	1710	rVB	49246	83517	3.03%	0.347%
28	12.212	1739	1744	1754	rBV3	23320	43878	1.59%	0.183%
29	12.312	1754	1761	1768	rBV	63363	107542	3.90%	0.447%
30	12.700	1822	1827	1834	rBV	27657	43054	1.56%	0.179%
31	12.859	1845	1854	1865	rBV	807496	1414803	51.26%	5.885%
32	13.041	1880	1885	1895	rVB	19898	33257	1.21%	0.138%
33	13.800	2006	2014	2024	rBV	758858	1308244	47.40%	5.442%
34	14.006	2043	2049	2056	rVB3	23268	42408	1.54%	0.176%

Sum of corrected areas: 24040568

Instrument :

MSVOA_N

ClientSampleId :

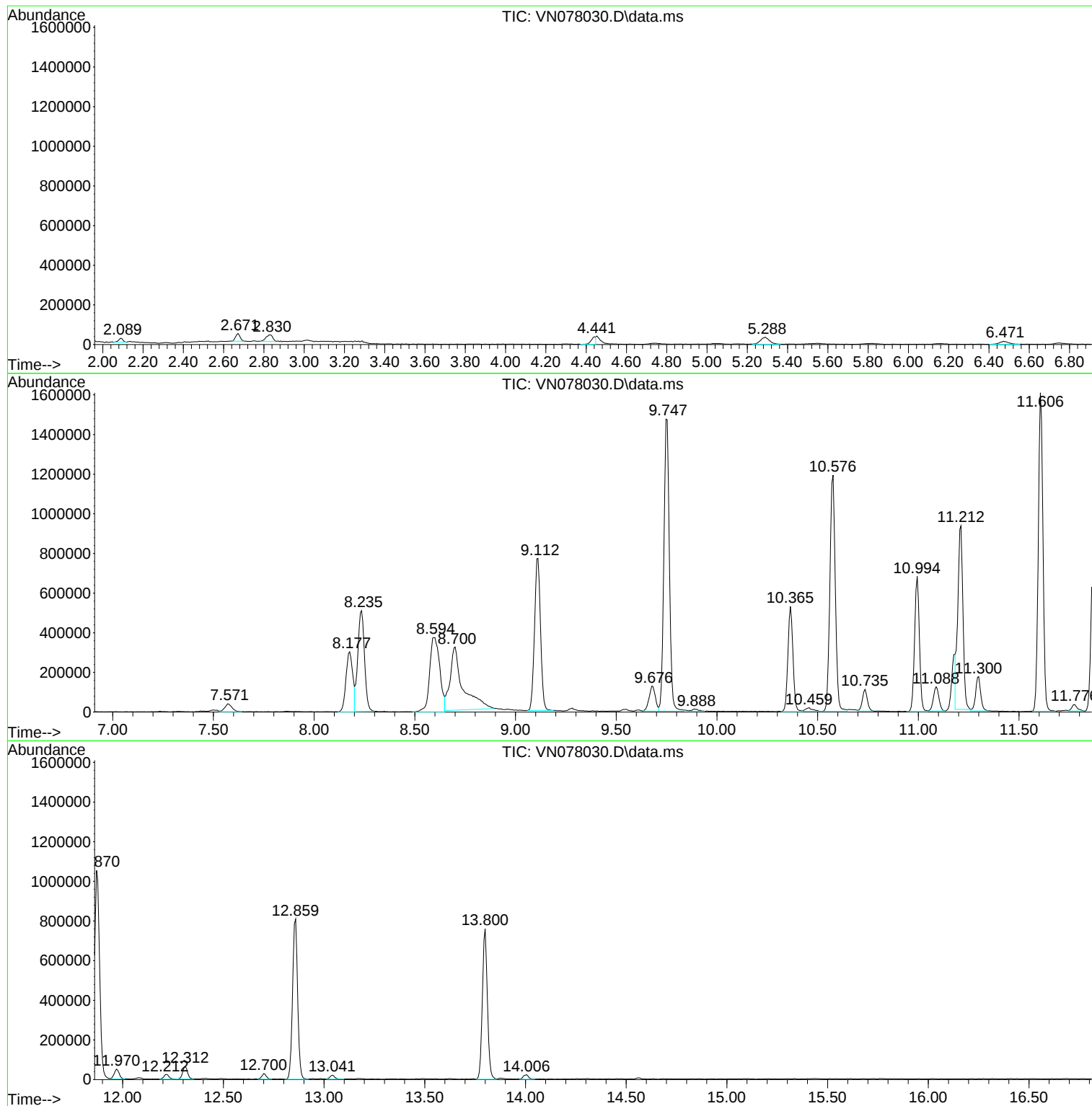
TP16-0A

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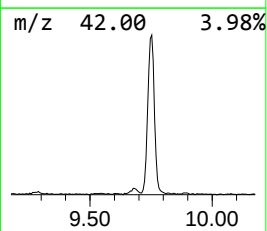
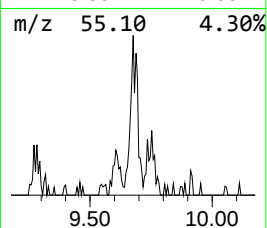
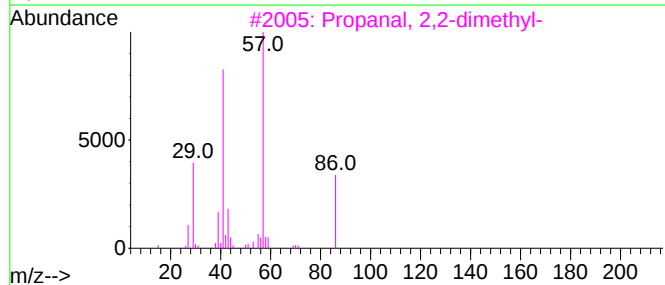
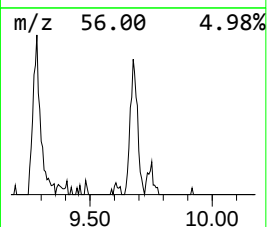
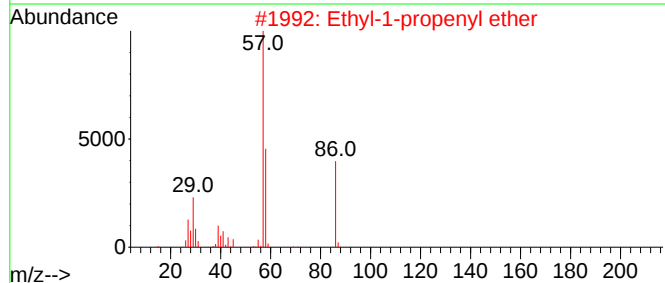
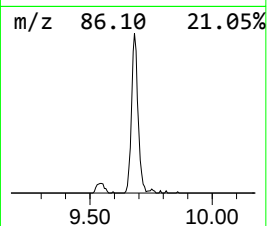
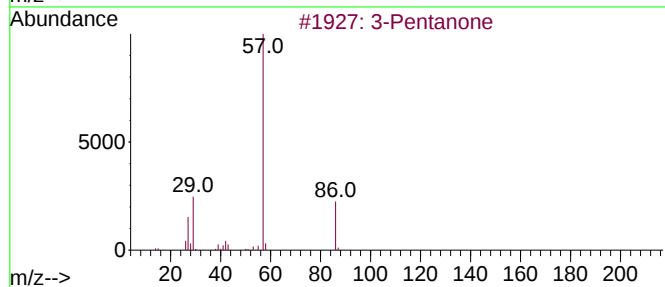
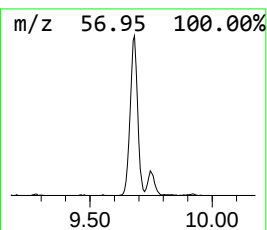
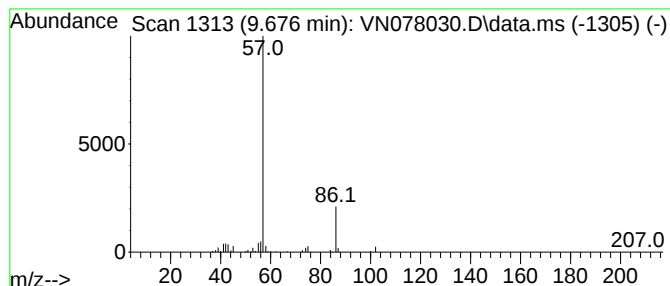
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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

Peak Number 1 3-Pentanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.676	8.70 ug/l	276106	1,4-Difluorobenzene	9.112

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanone	86	C5H10O	000096-22-0	64
2			Ethyl-1-propenyl ether	86	C5H10O	000928-55-2	53
3			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	9
4			Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	9
5			Thiolane-3,4-dicarbonitrile, 2,5...	386	C16H20F6N2S	1000260-74-6	9



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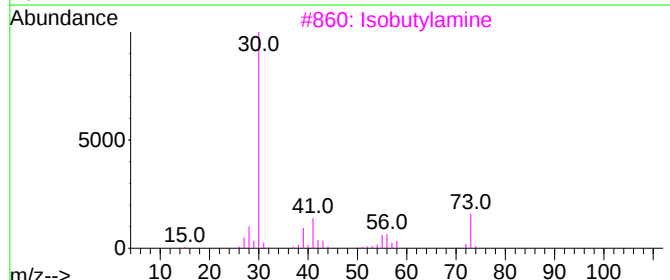
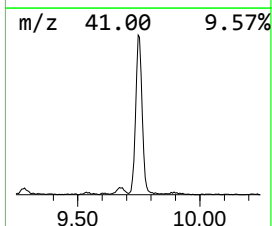
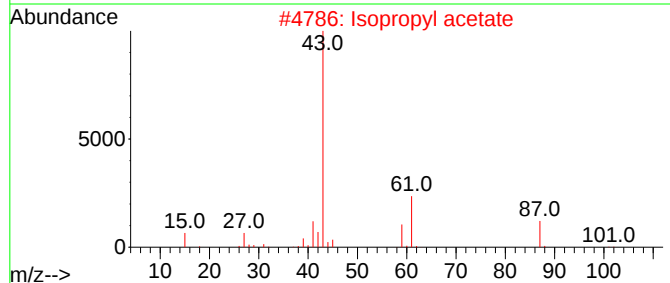
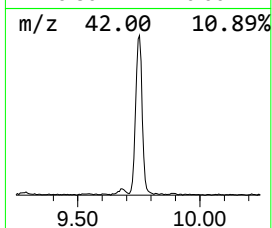
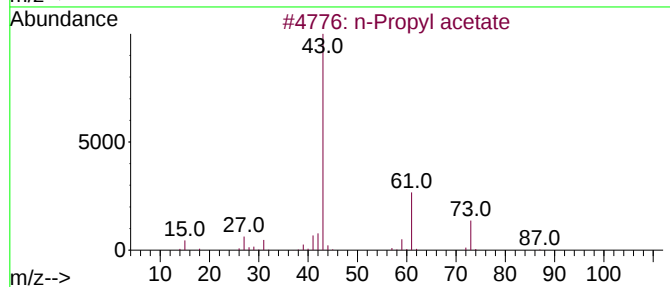
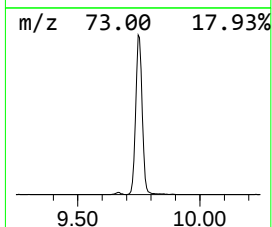
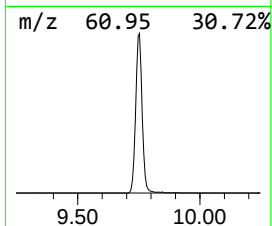
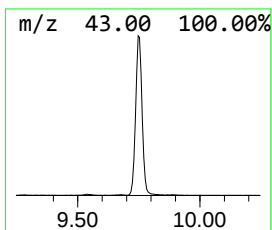
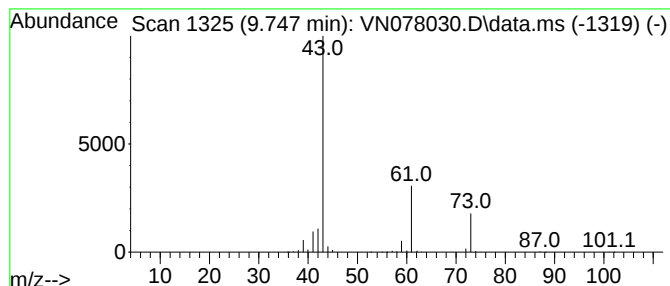
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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

Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.747	86.95 ug/l	2759910	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			Isobutylamine	73	C4H11N	000078-81-9	9
4			Isobutyl acetate	116	C6H12O2	000110-19-0	9
5			1-Butanamine	73	C4H11N	000109-73-9	7



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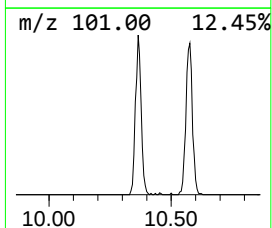
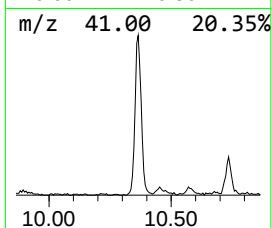
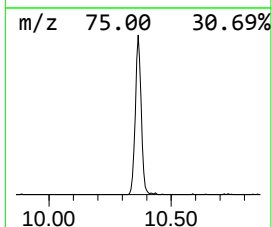
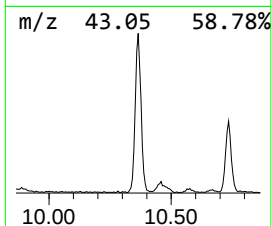
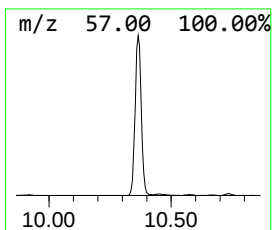
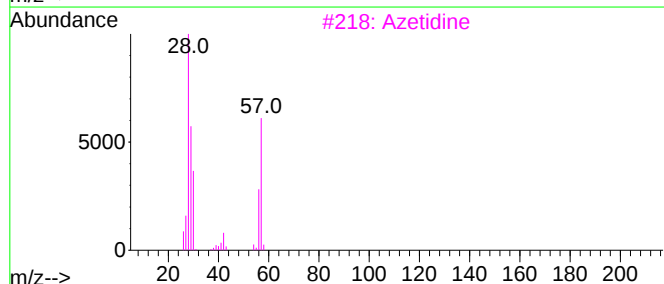
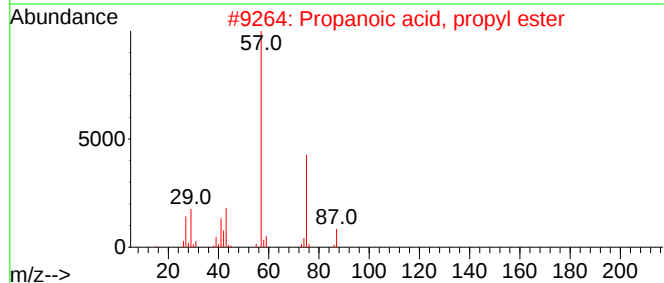
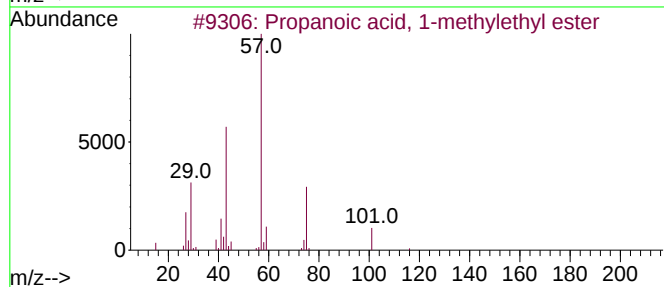
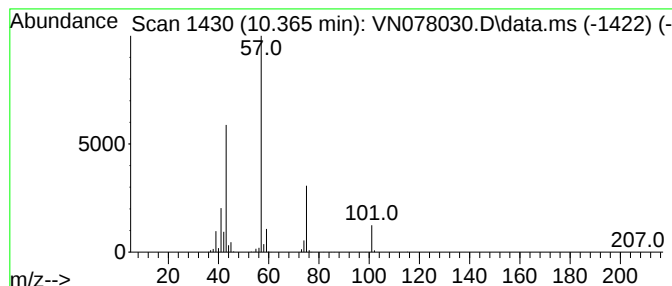
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.365	28.87 ug/l	916293	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			Azetidine	57	C3H7N	000503-29-7	12
4			Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	10
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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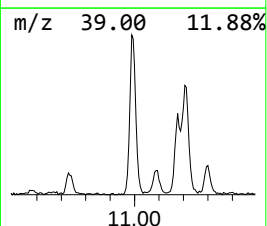
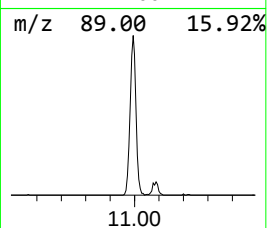
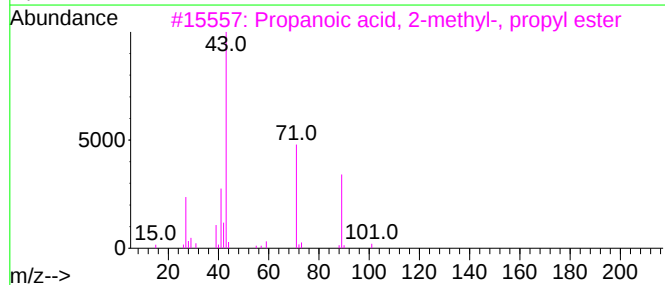
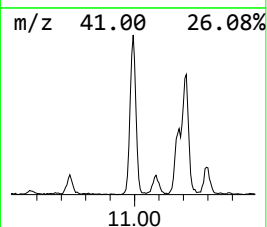
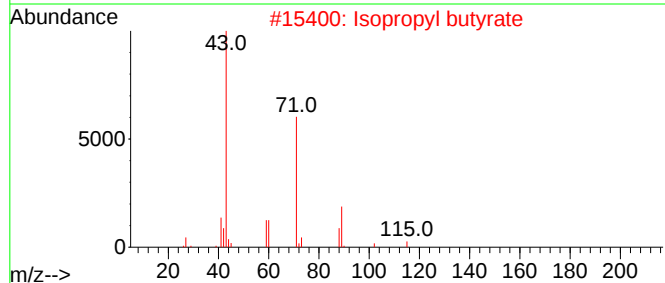
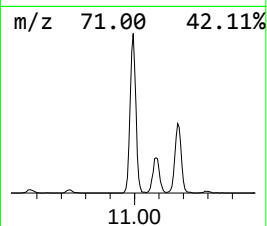
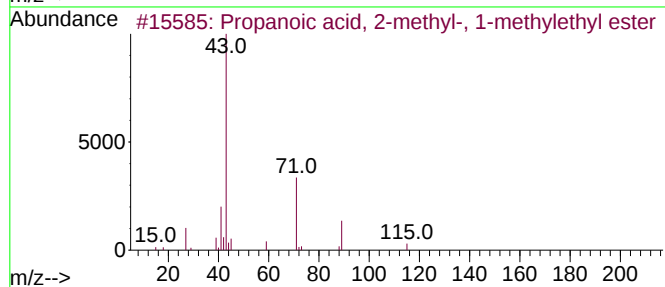
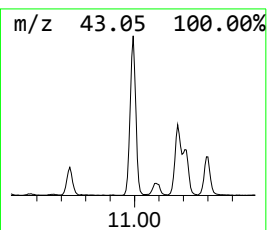
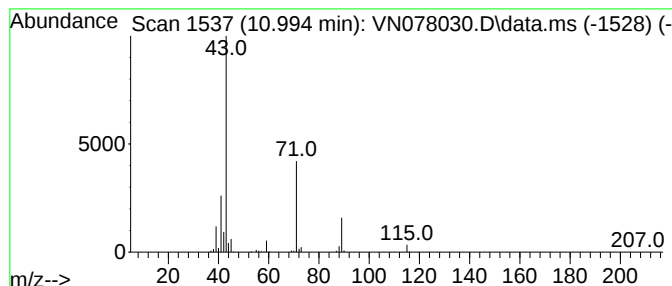
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Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.994	30.12 ug/l	1135920	Chlorobenzene-d5	11.870

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	64
4			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	45
5			Propanoic acid, 2-methyl-, 2-met...	172	C10H20O2	084254-82-0	39



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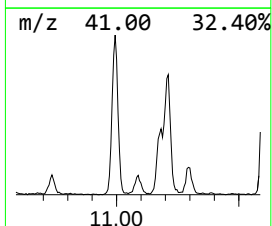
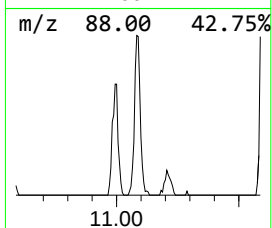
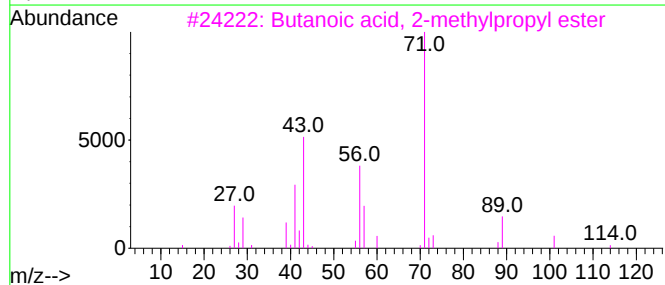
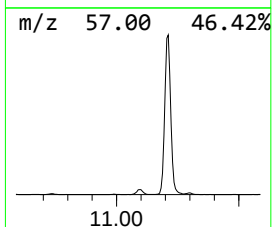
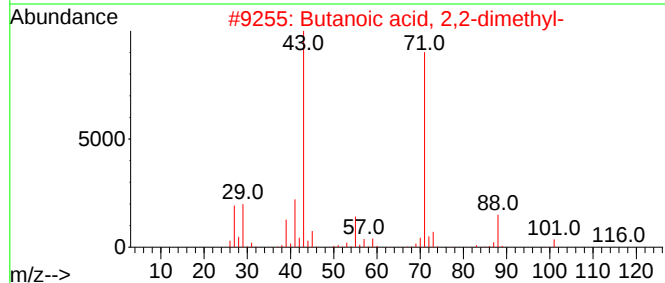
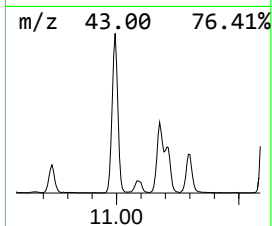
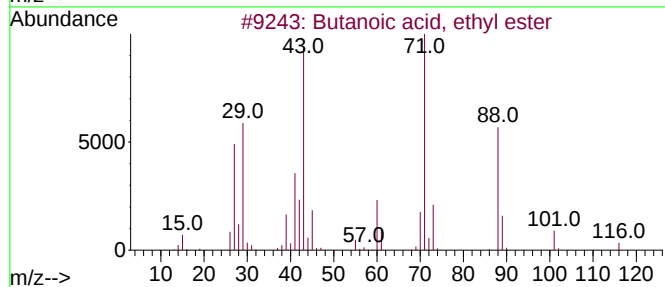
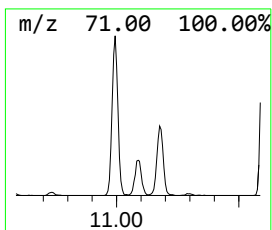
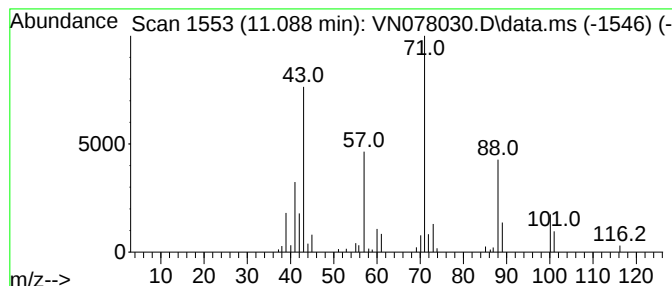
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Peak Number 5 Butanoic acid, ethyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.088	6.08 ug/l	229205	Chlorobenzene-d5	11.870

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	59
2			Butanoic acid, 2,2-dimethyl-	116	C6H12O2	000595-37-9	50
3			Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	50
4			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	43
5			Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	42



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TP16-0A

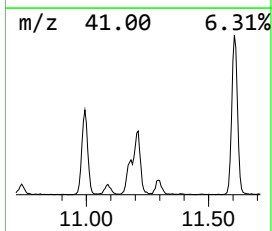
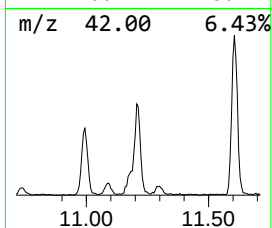
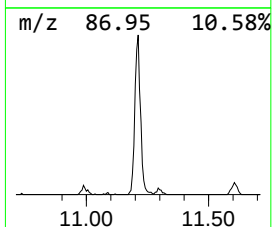
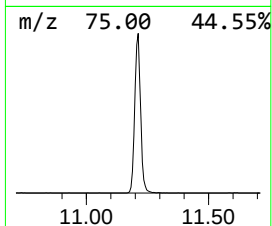
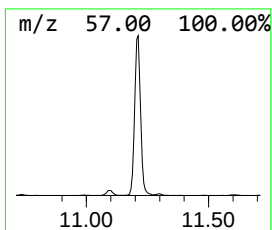
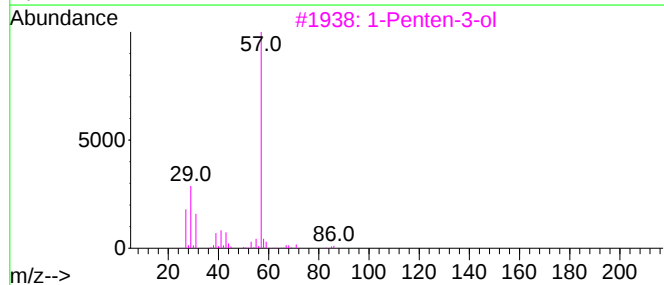
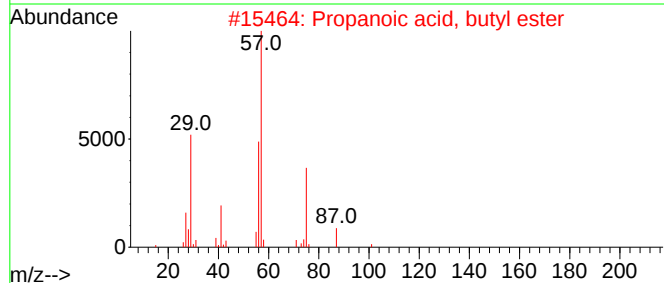
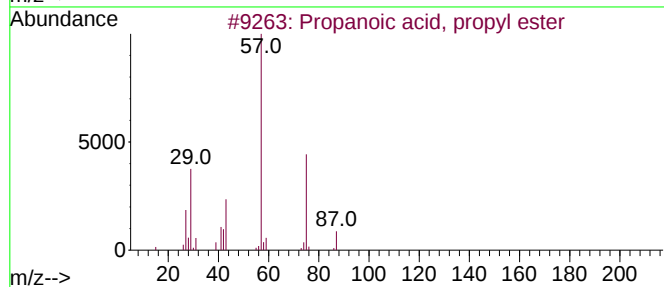
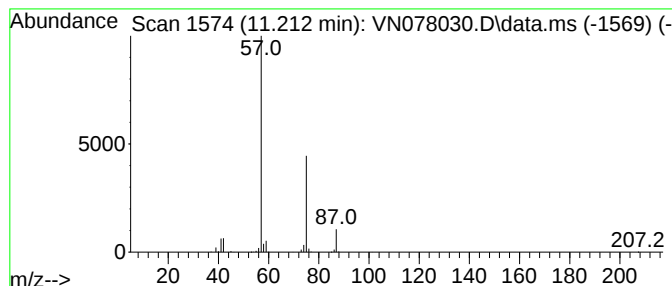
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Quant Title : SW846 8260

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.
11.212	43.35 ug/l	1634740	Chlorobenzene-d5	11.870

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	9
3			1-Penten-3-ol	86	C5H10O	000616-25-1	7
4			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	5
5			Neopentylamine	87	C5H13N	005813-64-9	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078030.D
Acq On : 02 Jun 2023 14:33
Operator : JC\MD
Sample : 03001-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP16-0A

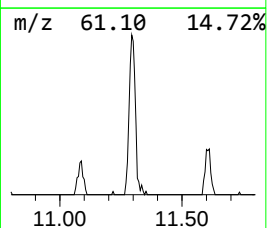
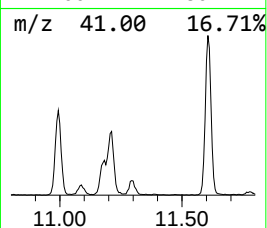
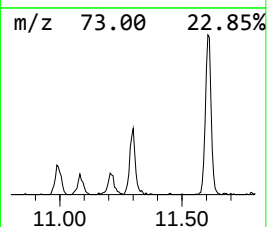
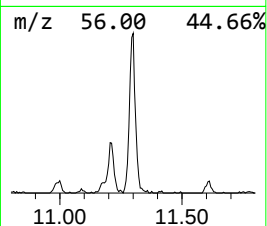
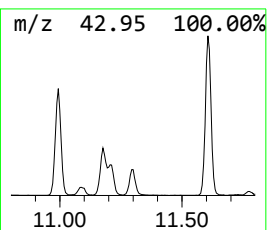
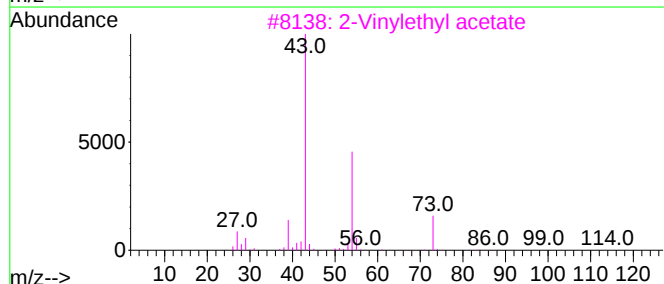
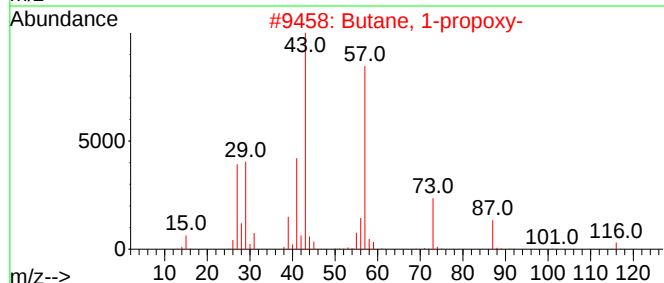
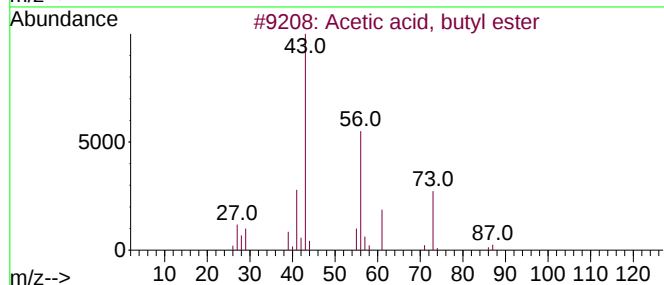
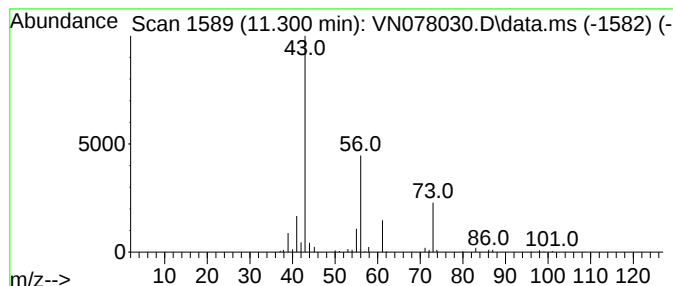
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Quant Title : SW846 8260

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

Peak Number 7 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.300	7.96 ug/l	300127	Chlorobenzene-d5	11.870

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2			Butane, 1-propoxy-	116	C7H16O	003073-92-5	25
3			2-Vinylethyl acetate	114	C6H10O2	001576-84-7	17
4			Isobutylamine	73	C4H11N	000078-81-9	9
5			Isopropyl pyruvate	130	C6H10O3	1000431-41-9	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078030.D
Acq On : 02 Jun 2023 14:33
Operator : JC\MD
Sample : 03001-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP16-0A

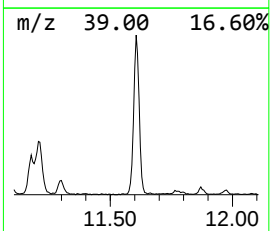
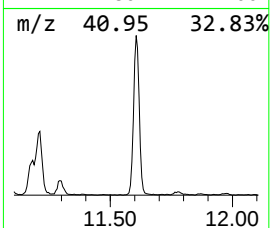
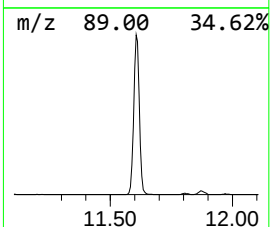
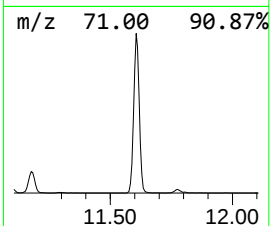
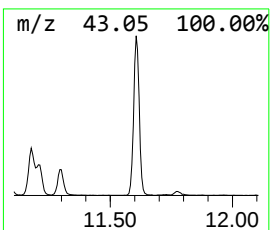
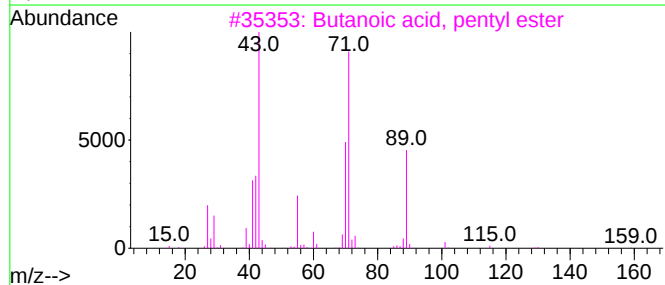
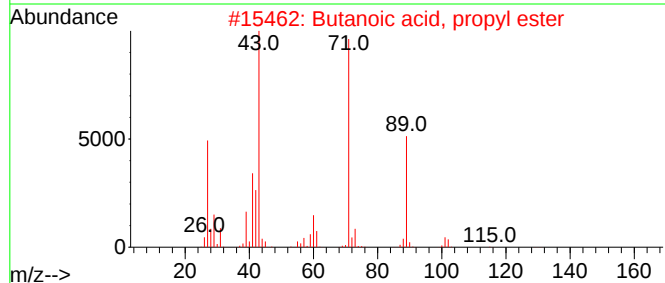
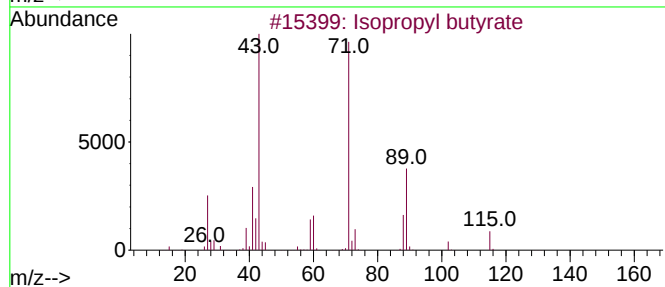
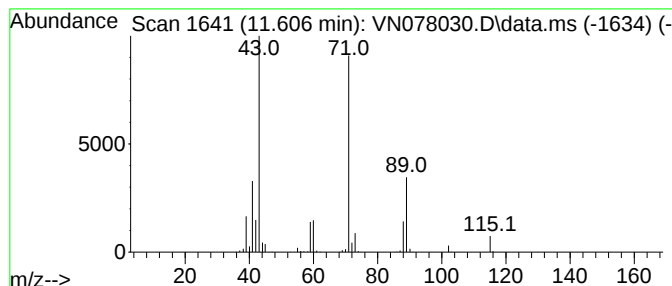
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Quant Title : SW846 8260

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	68.36 ug/l	2577970	Chlorobenzene-d5	11.870

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			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56
5			Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060223\
Data File : VN078030.D
Acq On : 02 Jun 2023 14:33
Operator : JC\MD
Sample : 03001-02
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP16-0A

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
3-Pentanone	9.676	8.7	ug/l	276106	2	9.112	1587080	50.0
n-Propyl acetate	9.747	87.0	ug/l	2759910	2	9.112	1587080	50.0
Propanoic acid,...	10.365	28.9	ug/l	916293	2	9.112	1587080	50.0
Propanoic acid,...	10.994	30.1	ug/l	1135920	3	11.870	1885490	50.0
Butanoic acid, ...	11.088	6.1	ug/l	229205	3	11.870	1885490	50.0
Propanoic acid,...	11.212	43.4	ug/l	1634740	3	11.870	1885490	50.0
Acetic acid, bu...	11.300	8.0	ug/l	300127	3	11.870	1885490	50.0
Isopropyl butyrate	11.606	68.4	ug/l	2577970	3	11.870	1885490	50.0