LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078060.D
Acq On : 05 Jun 2023 21:32
Operator : JC\MD
Sample : 03029-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-8

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: VN078060.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.824	140	148	155	rVB2	38843	89429	1.85%	0.303%
2	5.289	555	567	578	rBV3	18700	57384	1.18%	0.194%
3	7.571	949	955	966	rVB2	45546	107777	2.22%	0.365%
4	8.171	1047	1057	1062	rBV	309617	743491	15.35%	2.518%
5	8.230	1062	1067	1078	rVB	522279	1179654	24.35%	3.995%
6	8.588	1118	1128	1135	rBV	317601	714747	14.76%	2.421%
7	8.694	1135	1146	1158	rBV	313604	941039	19.43%	3.187%
8	9.106	1207	1216	1228	rBV	798826	1631692	33.69%	5.526%
9	9.677	1304	1313	1318	rBV2	131337	279010	5.76%	0.945%
10	9.747	1318	1325	1344	rVV	2635009	4843933	100.00%	16.405%
11	10.365	1422	1430	1439	rBV	600309	1013392	20.92%	3.432%
12	10.453	1439	1445	1456	rVB4	16455	51467	1.06%	0.174%
13	10.571	1456	1465	1477	rBV	1233092	2322256	47.94%	7.865%
14	10.735	1486	1493	1512	rVB	719159	1249435	25.79%	4.232%
15	10.994	1527	1537	1544	rBV	790533	1329512	27.45%	4.503%
16	11.088	1546	1553	1561	rVV3	152369	288317	5.95%	0.976%
17	11.206	1561	1573	1582	rVV2	1195673	2506919	51.75%	8.490%
18	11.294	1582	1588	1601	rVB	767398	1265290	26.12%	4.285%
19	11.606	1634	1641	1654	rBV	2322697	3660590	75.57%	12.398%
20	11.776	1664	1670	1678	rVB4	33793	65431	1.35%	0.222%
21	11.871	1678	1686	1697	rVV	1103171	1987813	41.04%	6.732%
22	11.965	1697	1702	1711	rVB2	27516	54733	1.13%	0.185%
23	12.212	1737	1744	1753	rBV2	26512	49879	1.03%	0.169%
24	12.312	1753	1761	1767	rBV2	160259	269426	5.56%	0.912%
25	12.853	1843	1853	1863	rBV	840663	1467256	30.29%	4.969%
26	13.800	2006	2014	2023	rBV	785045	1356519	28.00%	4.594%

Sum of corrected areas: 29526391

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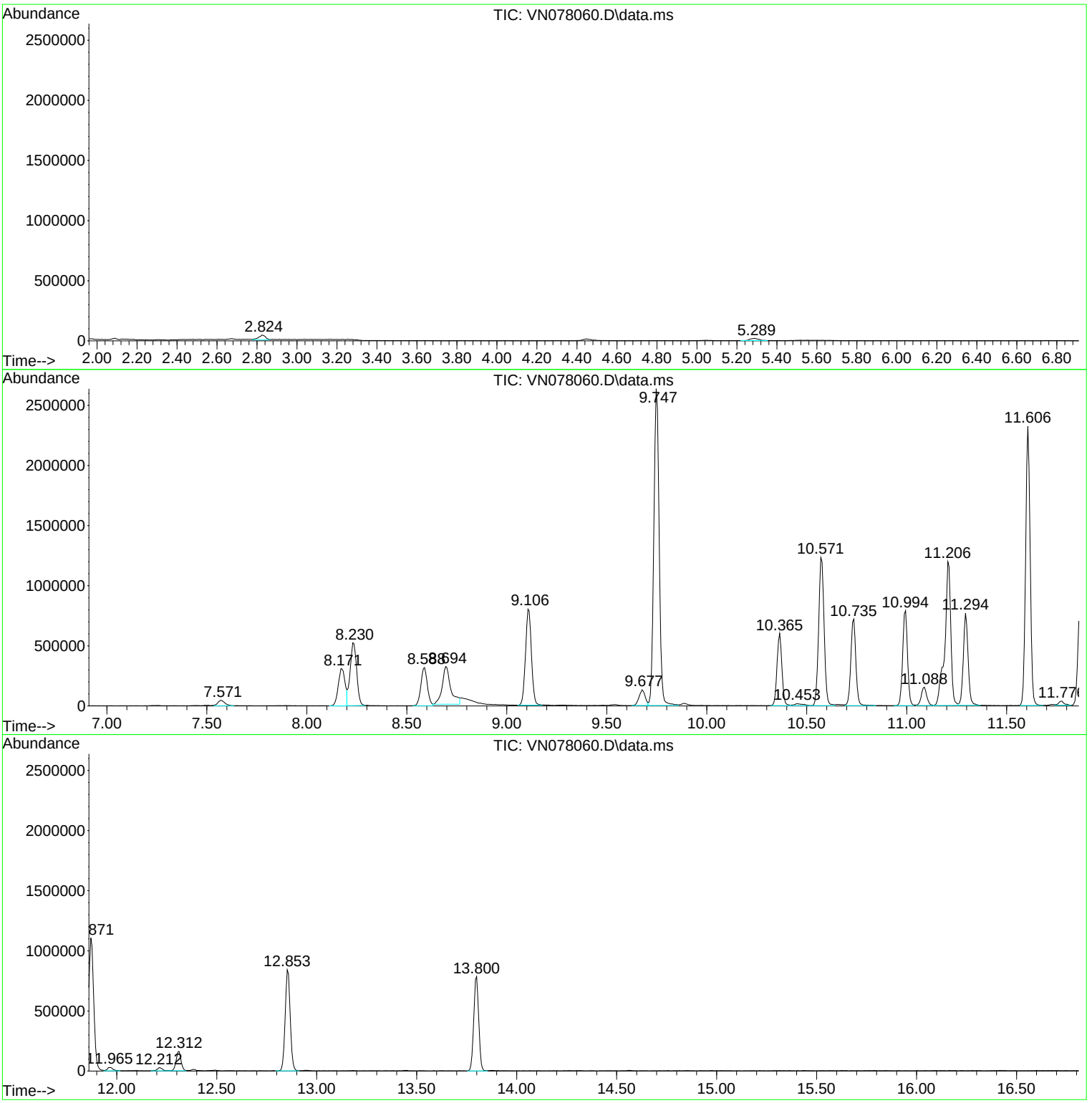
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

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



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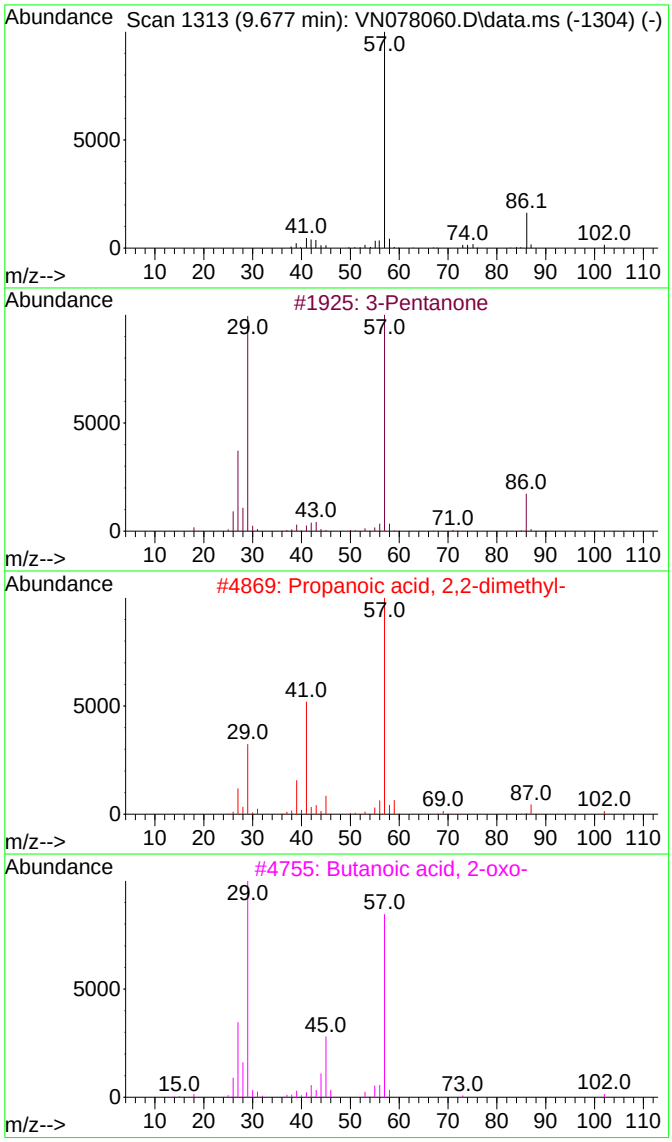
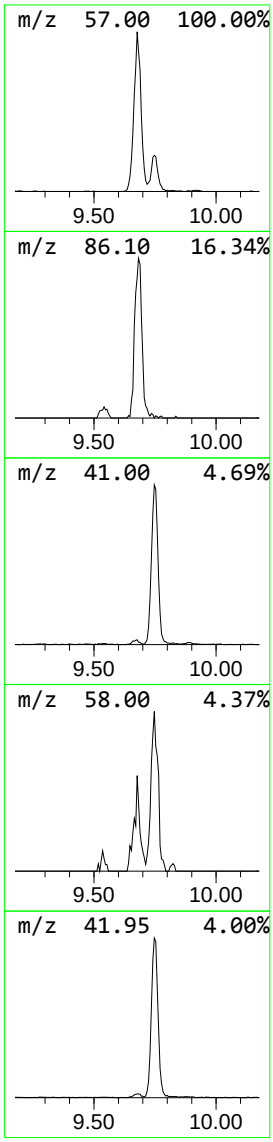
****
Peak Number 1 3-Pentanone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.677	8.55 ug/l	279010	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	80
2	Propanoic acid, 2,2-dimethyl-	102	C5H10O2	000075-98-9	25
3	Butanoic acid, 2-oxo-	102	C4H6O3	000600-18-0	9
4	2,2-Dimethyl-3-heptanone	142	C9H18O	019078-97-8	9
5	Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	9





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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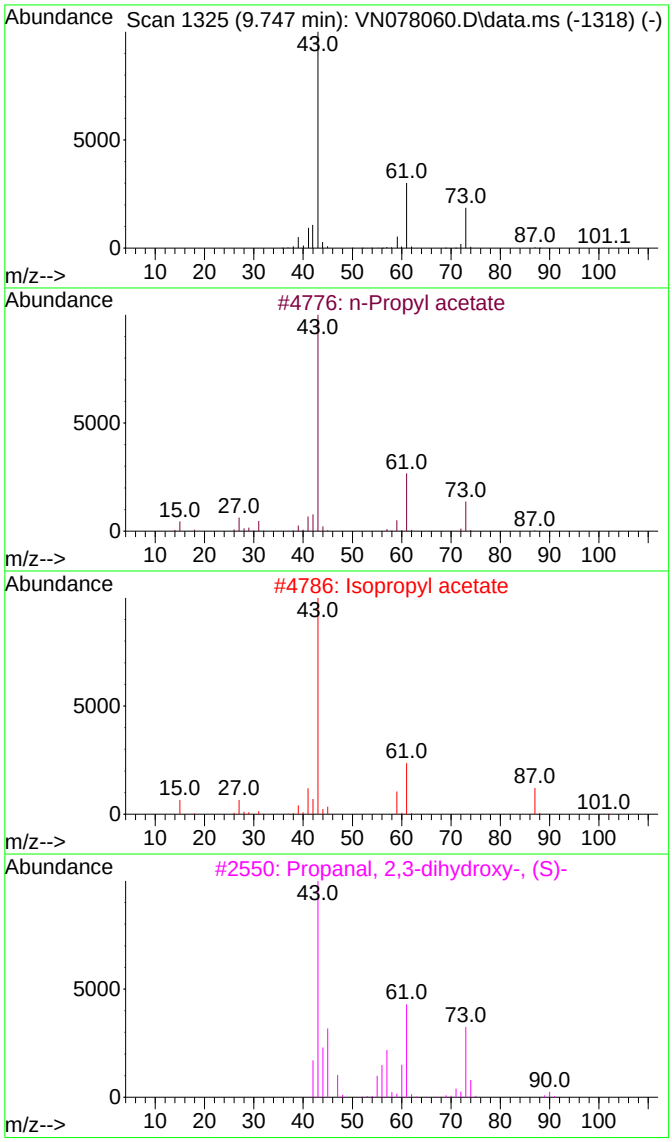
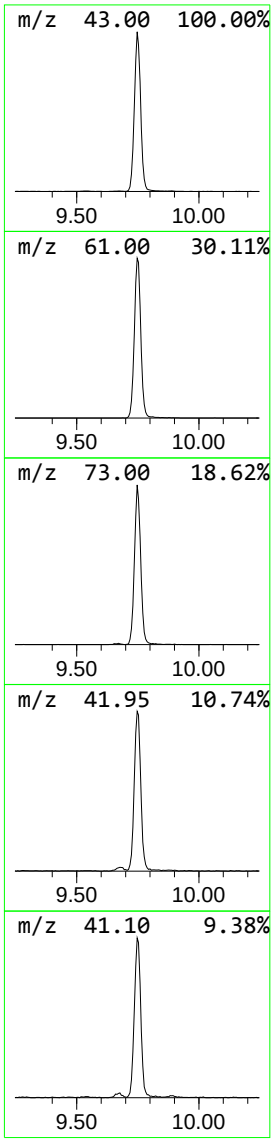
****
Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.747	148.43 ug/l	4843930	1,4-Difluorobenzene	9.106

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	36
4	Isobutyl acetate	116	C6H12O2	000110-19-0	9
5	1-Butanamine	73	C4H11N	000109-73-9	7





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
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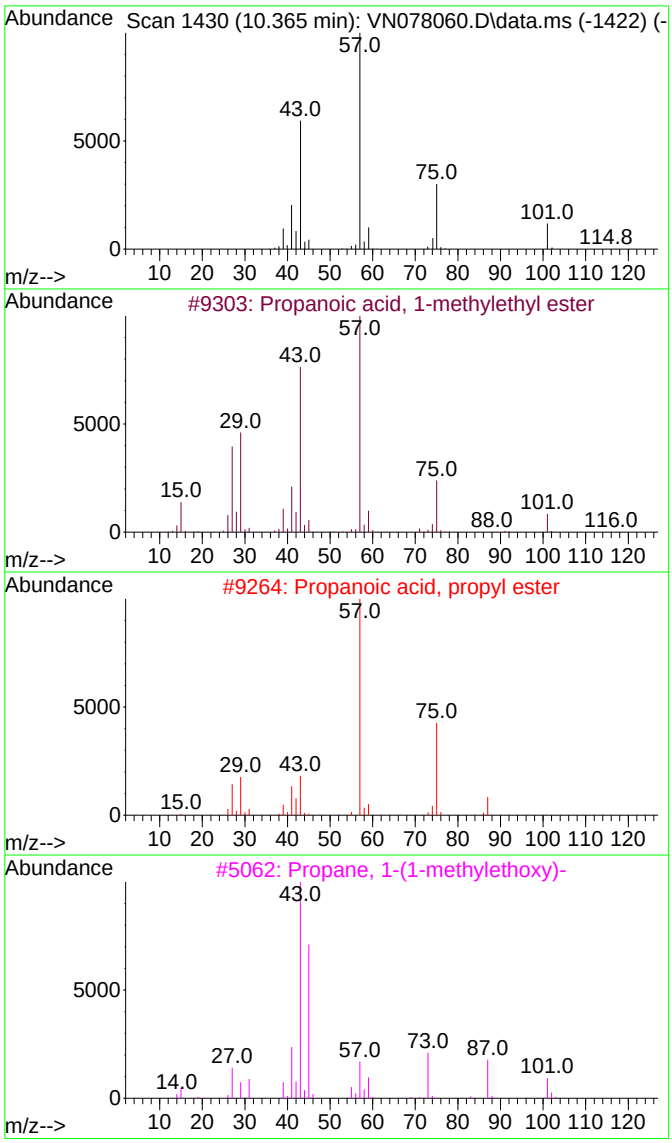
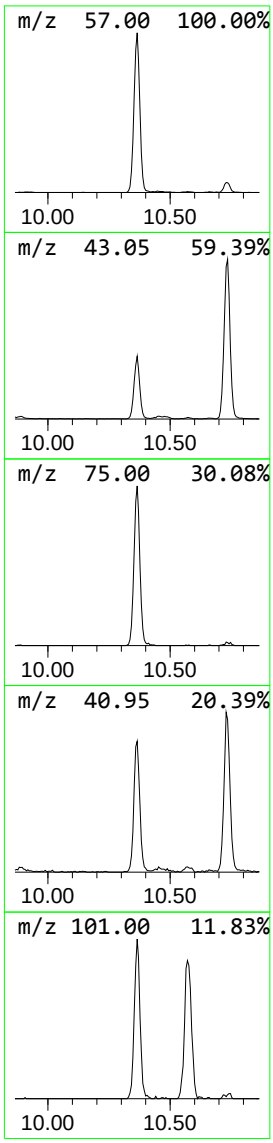
****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.365	31.05 ug/l	1013390	1,4-Difluorobenzene	9.106

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	42
3	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	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
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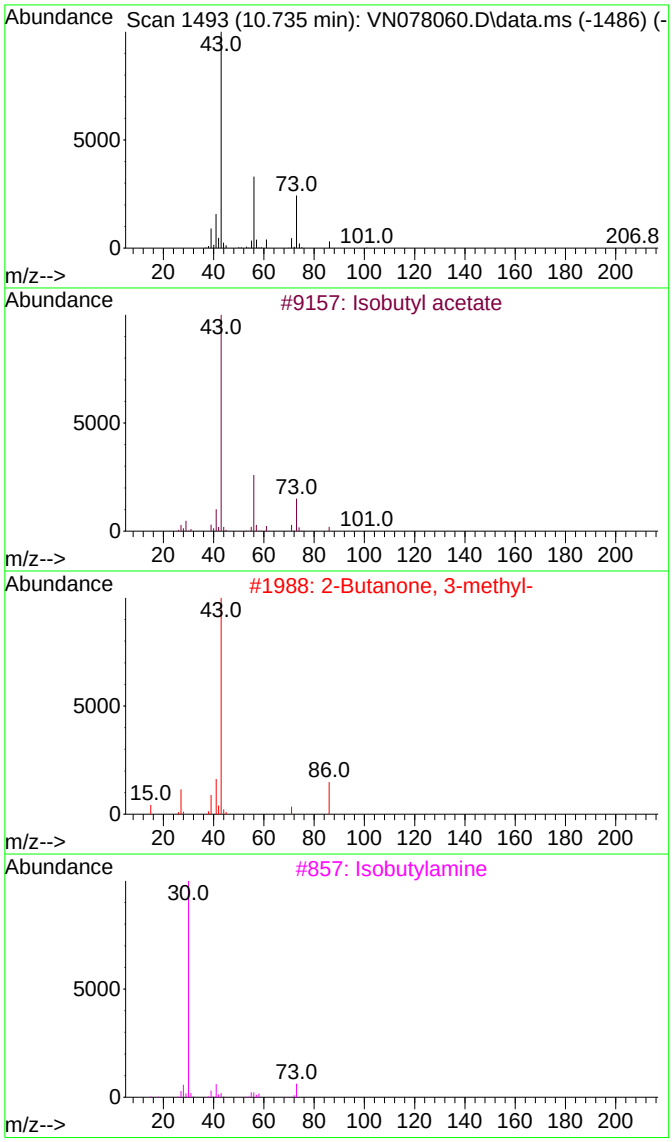
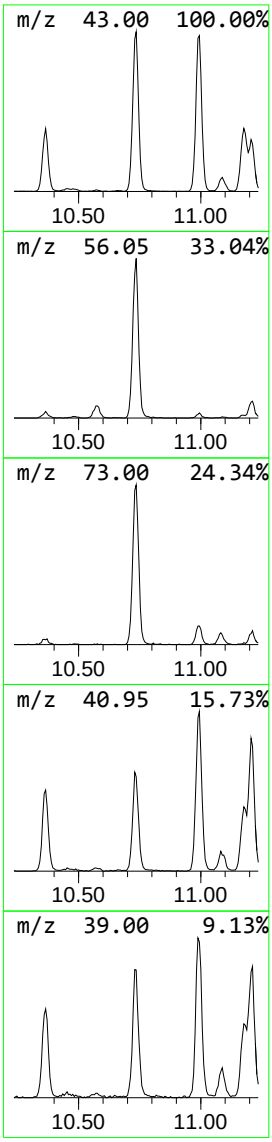
****
Peak Number 4 Isobutyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.735	31.43 ug/l	1249440	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	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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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
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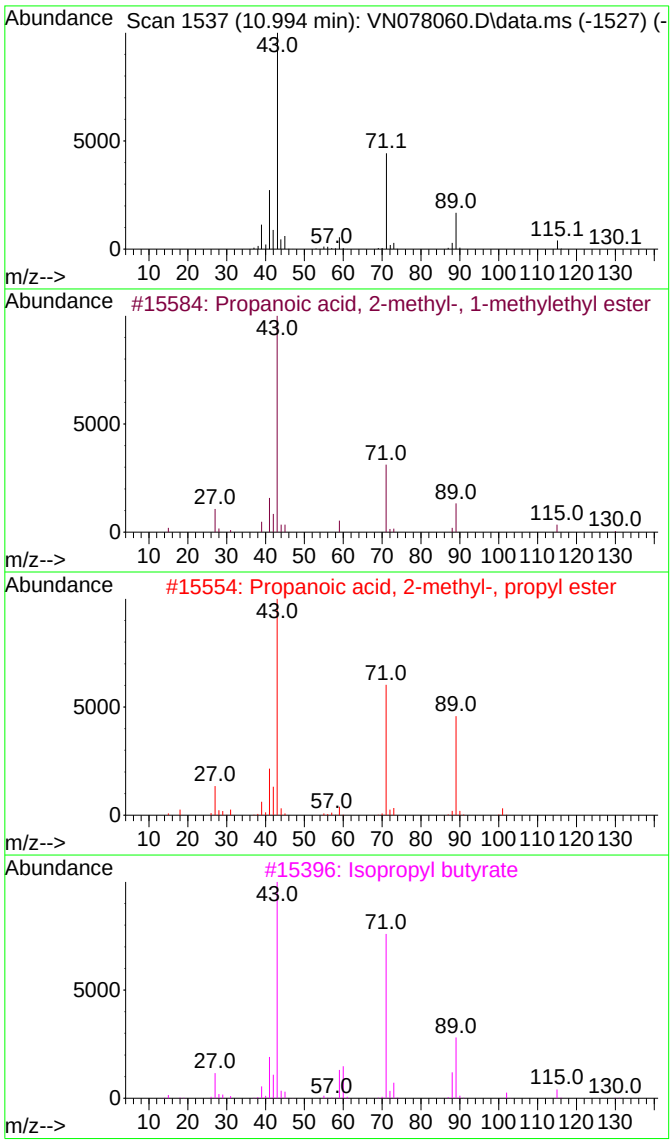
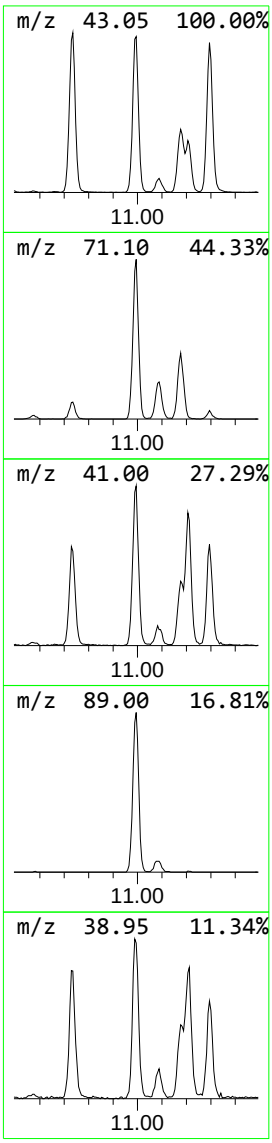
****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.994	33.44 ug/l	1329510	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	72
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	45
4	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	42
5	Propanoic acid, 2-methyl-, 2-met...	172	C10H20O2	084254-82-0	39





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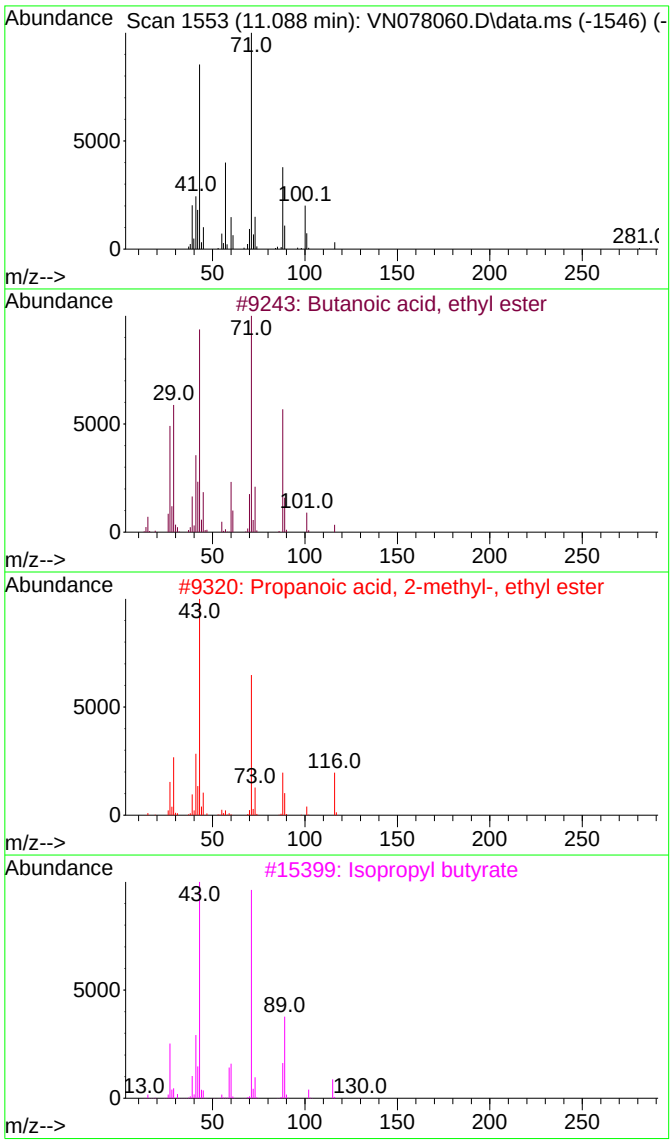
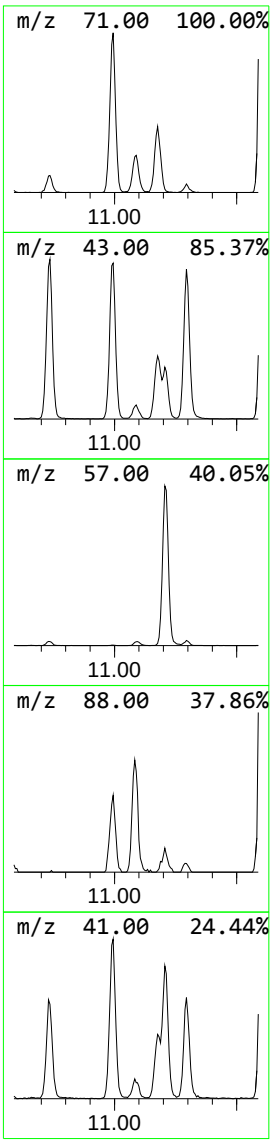
****
Peak Number 6 Butanoic acid, ethyl ester Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.088	7.25 ug/l	288317	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, ethyl ester	116	C6H12O2	000105-54-4	64
2	Propanoic acid, 2-methyl-, ethyl...	116	C6H12O2	000097-62-1	53
3	Isopropyl butyrate	130	C7H14O2	000638-11-9	50
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	40
5	Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	38





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TIC Library : C:\Database\NIST20.L
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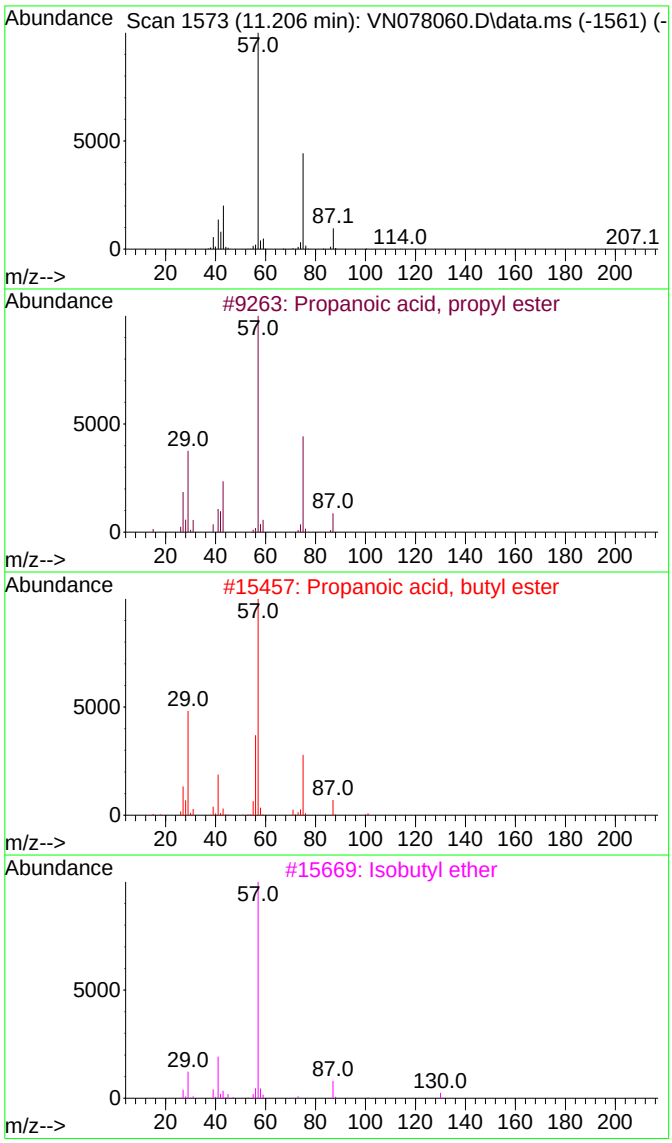
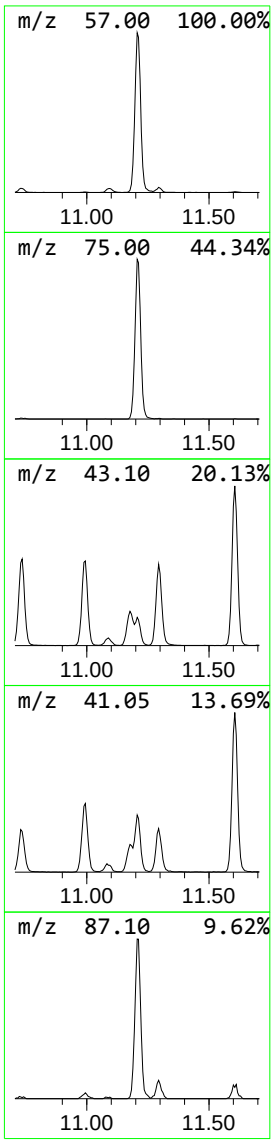
****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.206	63.06 ug/l	2506920	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	28
3	Isobutyl ether	130	C8H18O	000628-55-7	17
4	S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	9
5	2-(Isobutoxymethyl)oxirane	130	C7H14O2	003814-55-9	9





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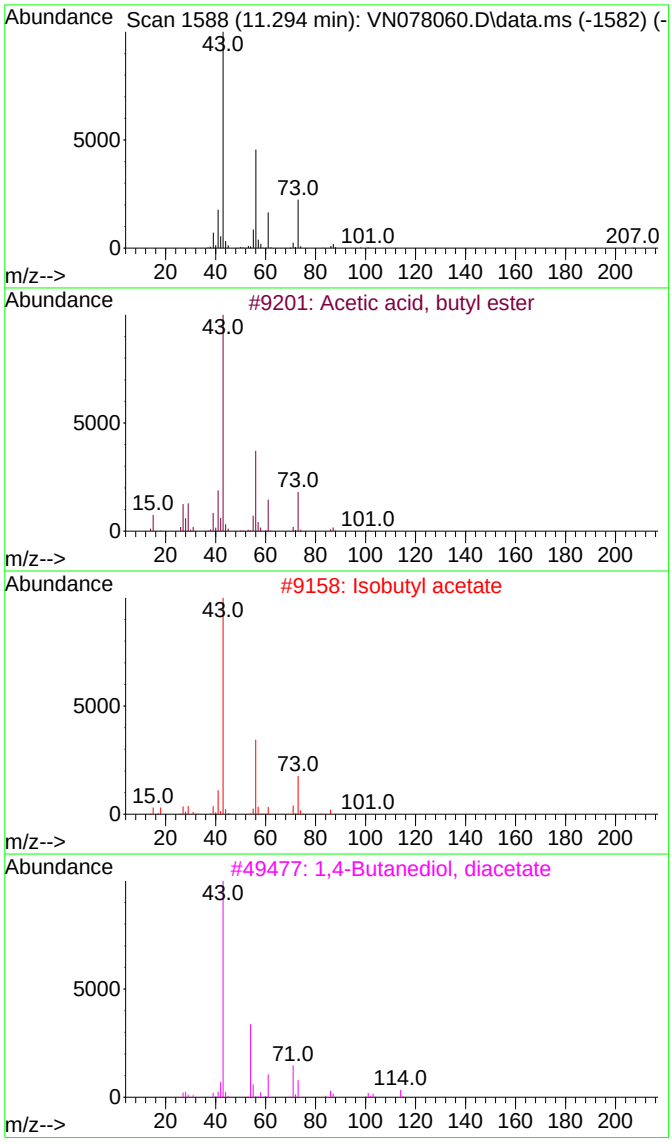
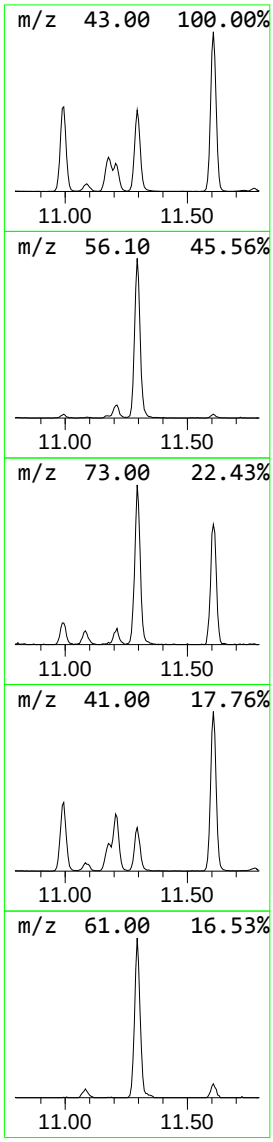
****
Peak Number 8 Acetic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.294	31.83 ug/l	1265290	Chlorobenzene-d5	11.871

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	Ethanol, 2-chloro-, acetate	122	C4H7ClO2	000542-58-5	9





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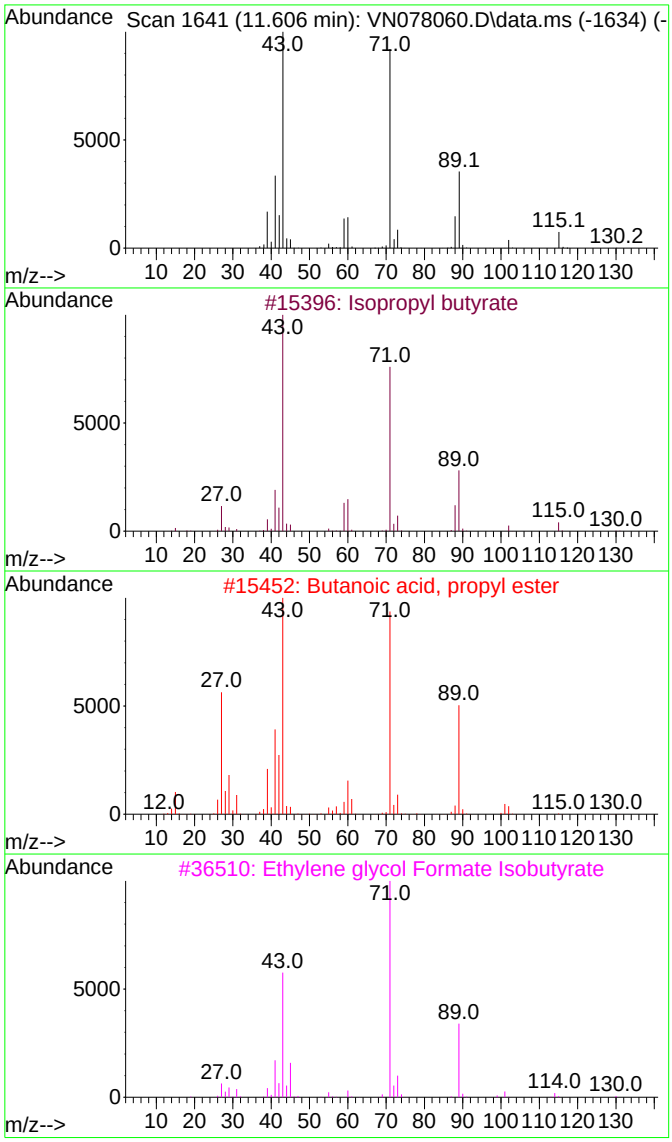
Quant Title : SW846 8260

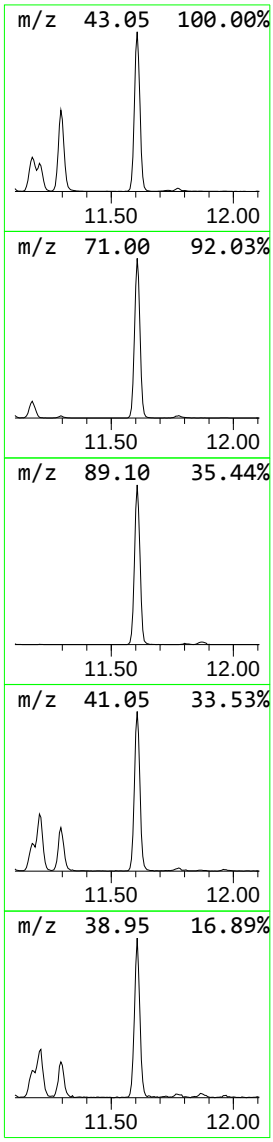
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Isopropyl butyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.606	92.08 ug/l	3660590	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	Ethylene glycol Formate Isobutyrate	160	C7H12O4	1000458-48-0	64
4	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
5	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	64





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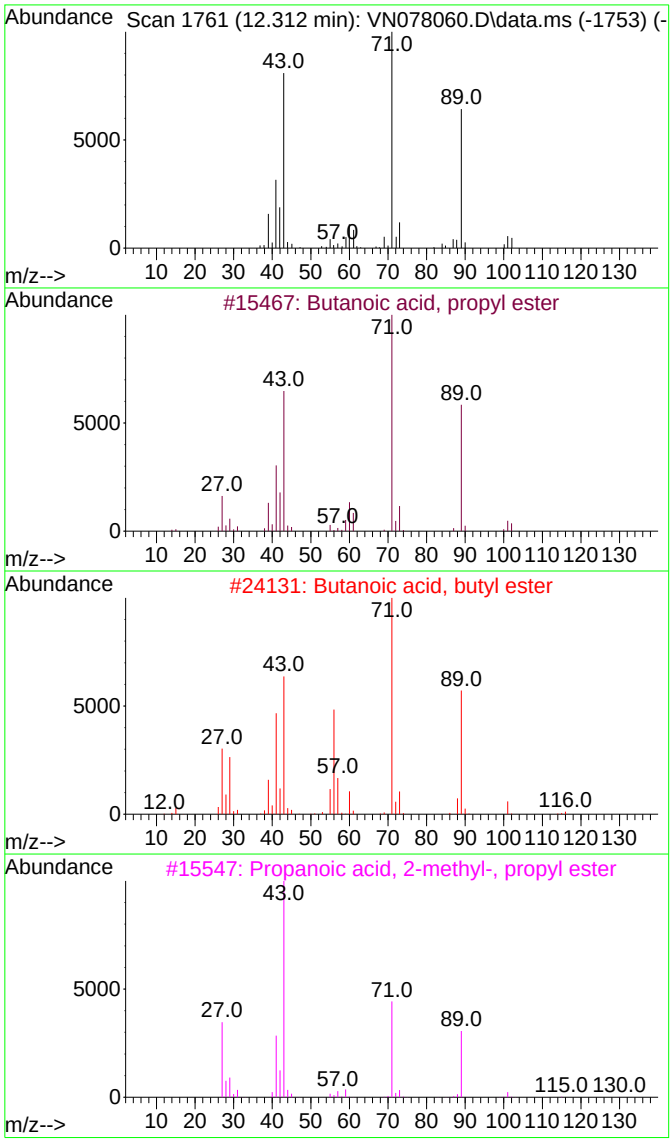
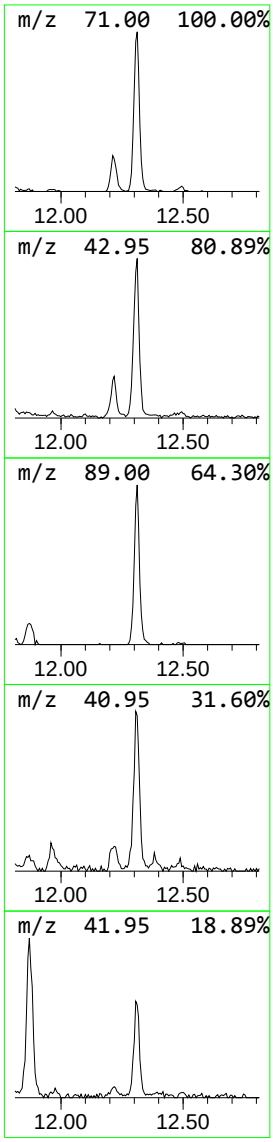
****
Peak Number 10 Butanoic acid, propyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.312	6.78 ug/l	269426	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	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	72
4	Propanoic acid, 2-methyl-, hexyl...	172	C10H20O2	002349-07-7	64
5	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078060.D
Acq On : 05 Jun 2023 21:32
Operator : JC\MD
Sample : 03029-08
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TP-8

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Pentanone	9.677	8.6	ug/l	279010	2	9.106	1631690	50.0
n-Propyl acetate	9.747	148.4	ug/l	4843930	2	9.106	1631690	50.0
Propanoic acid,...	10.365	31.1	ug/l	1013390	2	9.106	1631690	50.0
Isobutyl acetate	10.735	31.4	ug/l	1249440	3	11.871	1987810	50.0
Propanoic acid,...	10.994	33.4	ug/l	1329510	3	11.871	1987810	50.0
Butanoic acid, ...	11.088	7.3	ug/l	288317	3	11.871	1987810	50.0
Propanoic acid,...	11.206	63.1	ug/l	2506920	3	11.871	1987810	50.0
Acetic acid, bu...	11.294	31.8	ug/l	1265290	3	11.871	1987810	50.0
Isopropyl butyrate	11.606	92.1	ug/l	3660590	3	11.871	1987810	50.0
Butanoic acid, ...	12.312	6.8	ug/l	269426	3	11.871	1987810	50.0