LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN060523\
Data File : VN078057.D
Acq On : 05 Jun 2023 20:21
Operator : JC\MD
Sample : 03018-14
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RT-4648

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: VN078057.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	137	148	155	rBV2	33086	79336	2.86%	0.398%
2	4.453	415	425	433	rBV2	10765	34108	1.23%	0.171%
3	5.283	556	566	579	rBV3	19793	64132	2.31%	0.322%
4	7.577	949	956	968	rVB2	33770	82856	2.98%	0.416%
5	8.171	1045	1057	1062	rBV	310086	740527	26.65%	3.715%
6	8.230	1062	1067	1079	rVB	514522	1167314	42.01%	5.856%
7	8.588	1114	1128	1137	rBV	313305	716671	25.79%	3.595%
8	8.694	1137	1146	1157	rBV	224289	606815	21.84%	3.044%
9	9.106	1208	1216	1234	rVB	770603	1617867	58.22%	8.117%
10	9.677	1303	1313	1318	rBV	88663	189890	6.83%	0.953%
11	9.747	1318	1325	1341	rVV	1507835	2778781	100.00%	13.941%
12	10.365	1420	1430	1441	rBV	385540	675919	24.32%	3.391%
13	10.571	1456	1465	1479	rBV	1199188	2270537	81.71%	11.391%
14	10.735	1486	1493	1503	rVB	372884	637681	22.95%	3.199%
15	10.994	1529	1537	1547	rBV	443424	745808	26.84%	3.742%
16	11.088	1547	1553	1561	rVV3	63057	121151	4.36%	0.608%
17	11.177	1561	1568	1569	rVV	199451	279247	10.05%	1.401%
18	11.206	1569	1573	1581	rVV	428223	792410	28.52%	3.975%
19	11.294	1581	1588	1598	rVB	206871	357460	12.86%	1.793%
20	11.606	1633	1641	1653	rBV	851748	1393195	50.14%	6.990%
21	11.771	1665	1669	1678	rVB2	17464	29196	1.05%	0.146%
22	11.871	1678	1686	1698	rVB	1069448	1918391	69.04%	9.624%
23	12.312	1755	1761	1767	rVV2	25221	43721	1.57%	0.219%
24	12.853	1846	1853	1864	rBV	772885	1362200	49.02%	6.834%
25	13.794	2006	2013	2024	rBV	715030	1227246	44.16%	6.157%

Sum of corrected areas: 19932459

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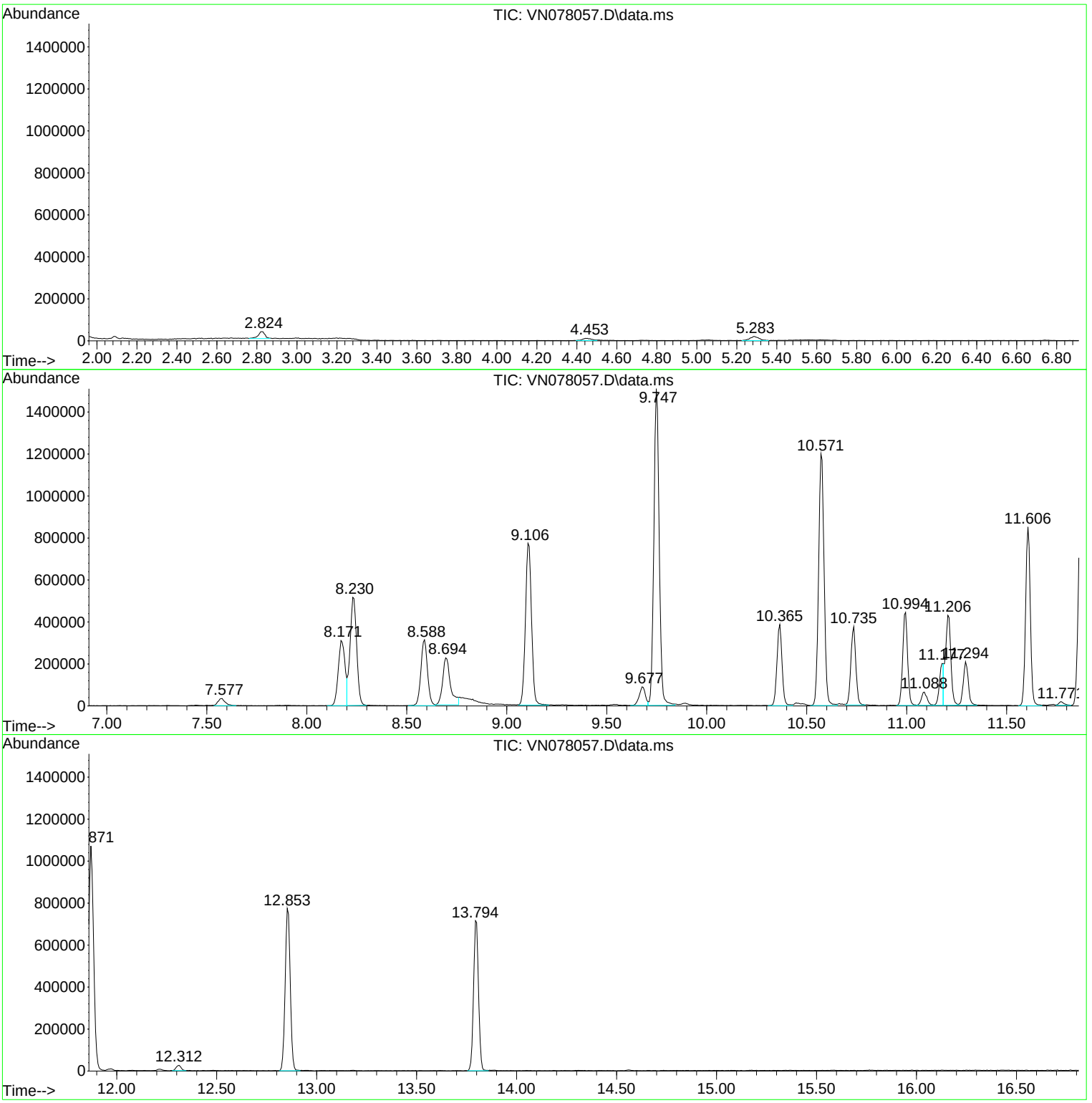
RT-4648

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 Title : SW846 8260

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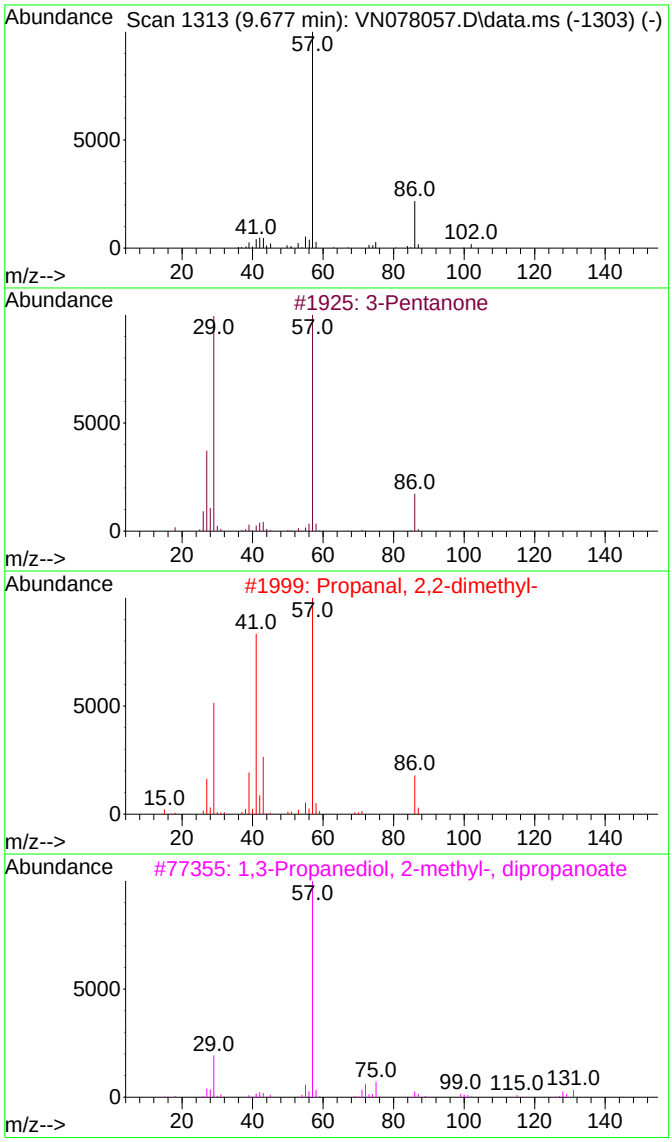
TIC Integration Parameters: LSCINT.P

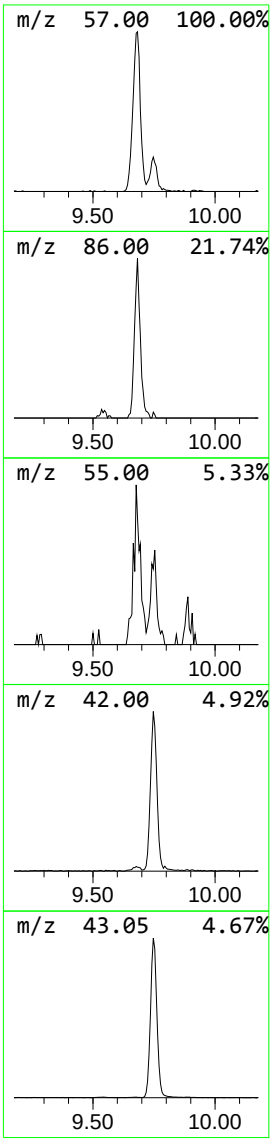
****

Peak Number 1 3-Pentanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.677	5.87 ug/l	189890	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	72
2	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	38
3	1,3-Propanediol, 2-methyl-, dipr...	202	C10H18O4	054932-83-1	25
4	Butanoic acid, 2-oxo-	102	C4H6O3	000600-18-0	25
5	1,5-Hexadien-3-ol	98	C6H10O	000924-41-4	23





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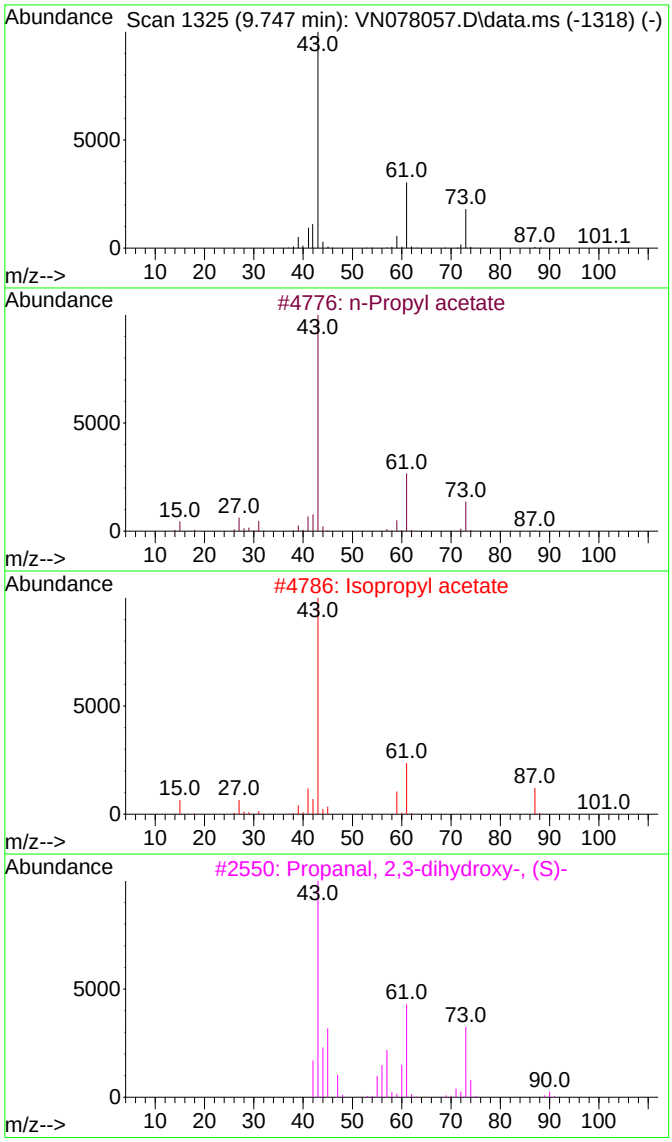
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

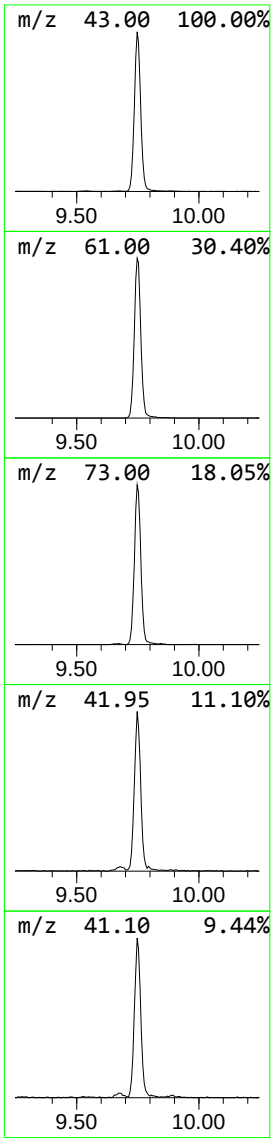
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.747	85.88 ug/l	2778780	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	9
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
Quant Title : SW846 8260

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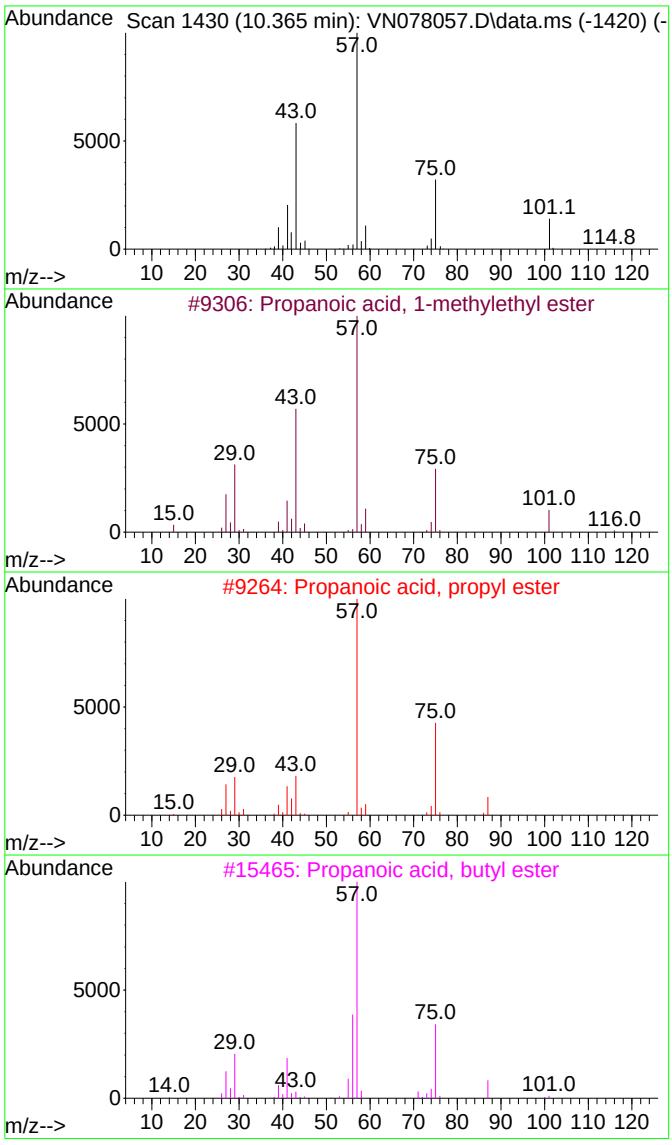
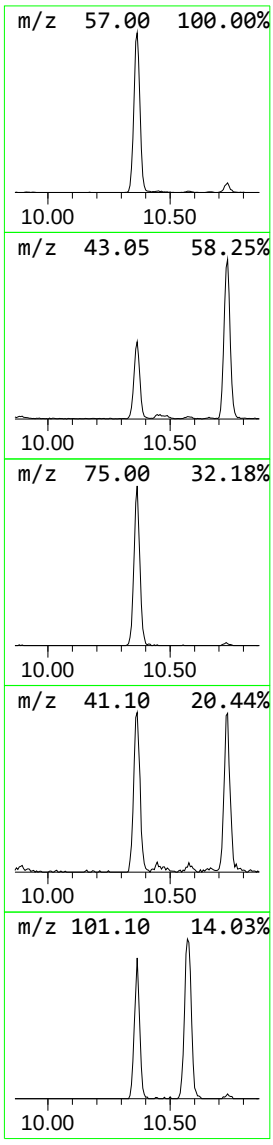
****
Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.365	20.89 ug/l	675919	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	90
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	53
3	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	38
4	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	10
5	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	9





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Instrument :
MSVOA_N
ClientSampleId :
RT-4648

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

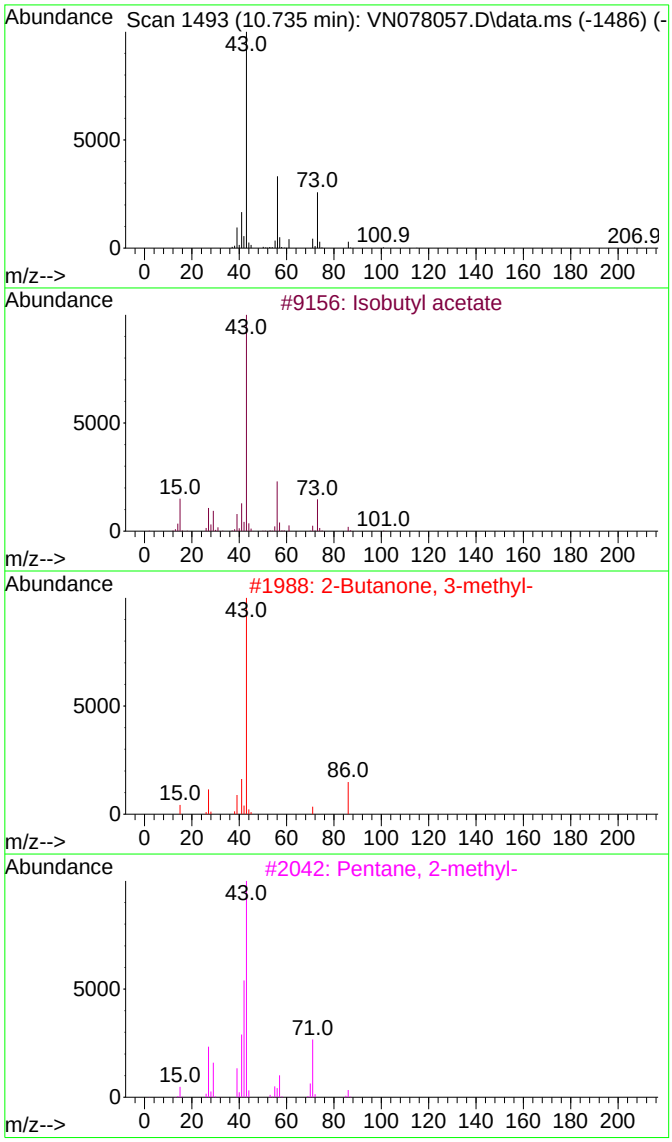
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

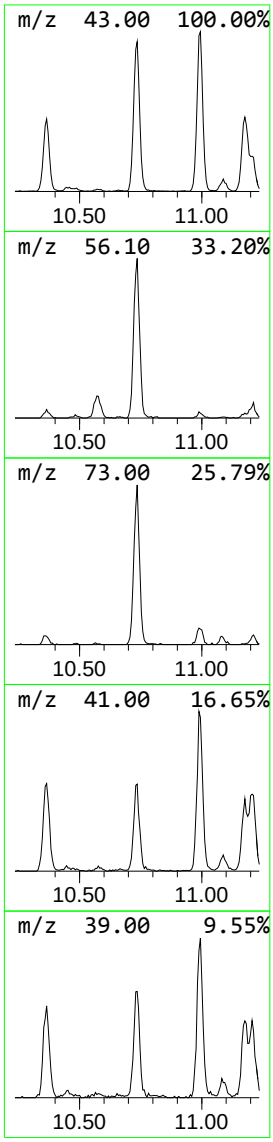
****

Peak Number 4 Isobutyl acetate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.735	16.62 ug/l	637681	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	Isobutylamine	73	C4H11N	000078-81-9	9
5	Acetic acid, butyl ester	116	C6H12O2	000123-86-4	9





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Instrument :
MSVOA_N
ClientSampleId :
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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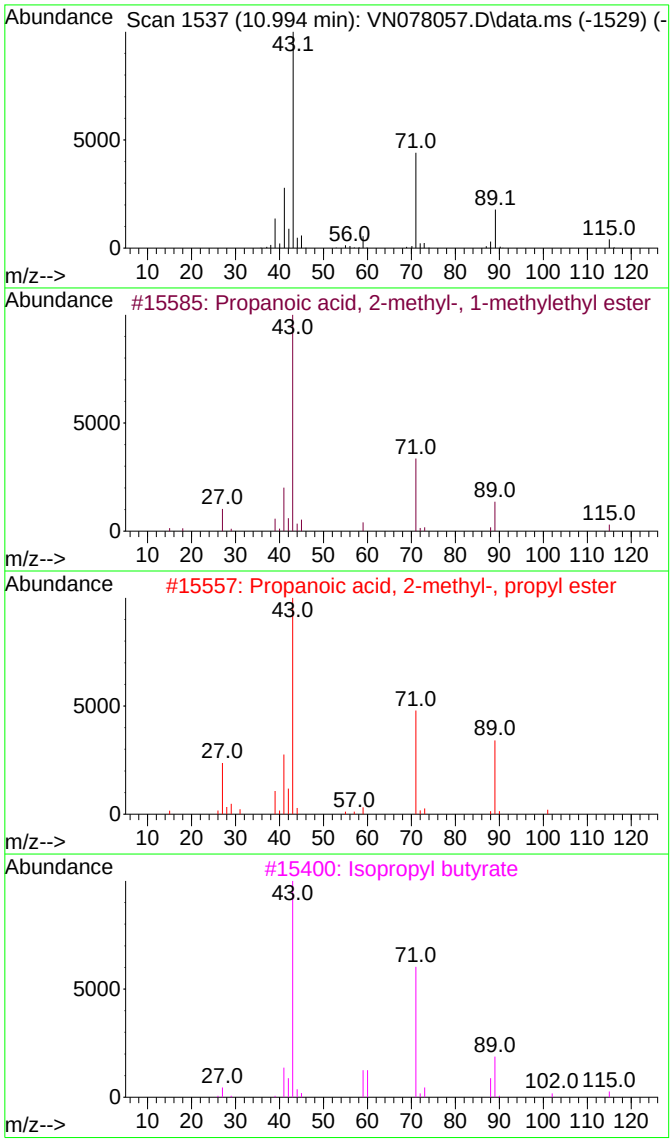
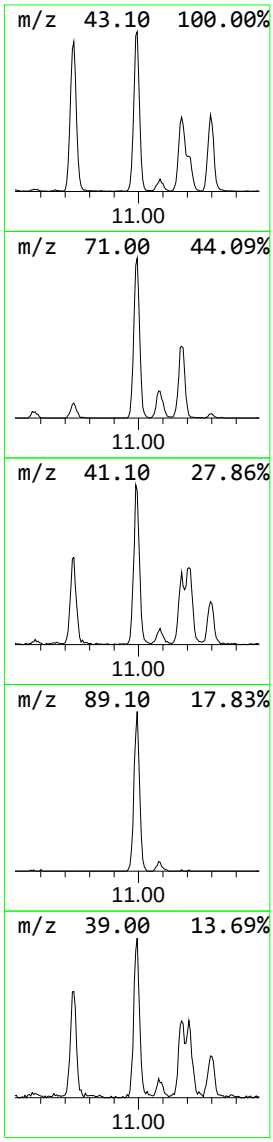
****
Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.994	19.44 ug/l	745808	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	72
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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MSVOA_N
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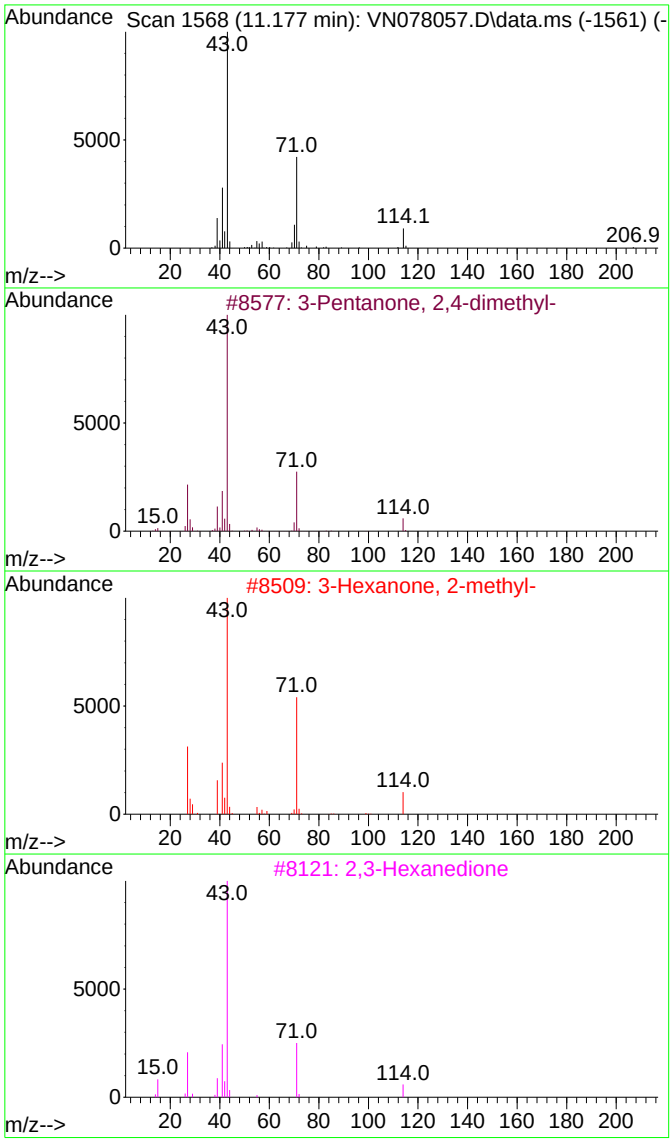
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

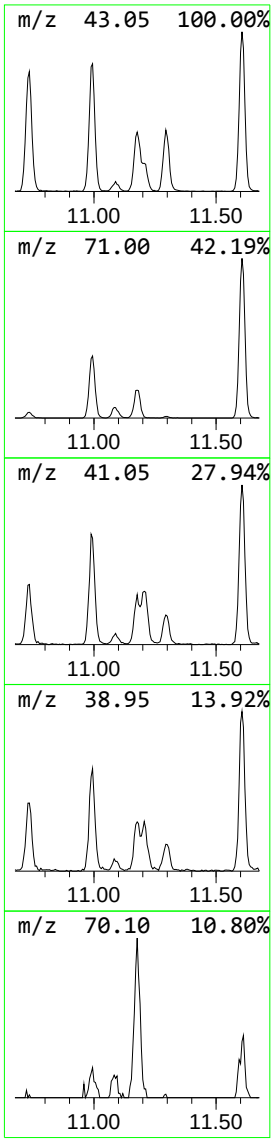
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 3-Pentanone, 2,4-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.177	7.28 ug/l	279247	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	86
2	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	72
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	64
4	4-Heptanone	114	C7H14O	000123-19-3	53
5	Azetidine, 1-methyl-	71	C4H9N	004923-79-9	50





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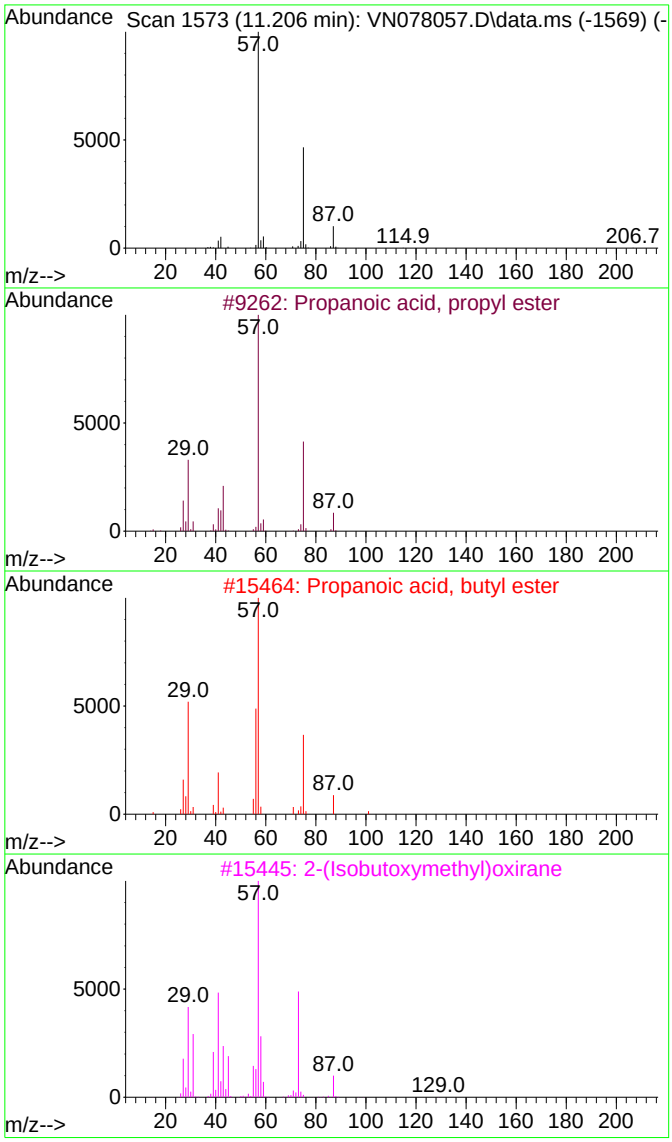
Quant Title : SW846 8260

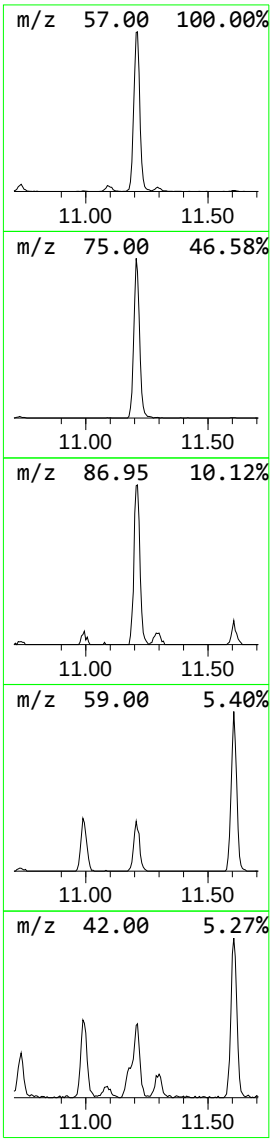
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Propanoic acid, propyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.206	20.65 ug/l	792410	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	1-Pentanamine	87	C5H13N	000110-58-7	7
5	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	5





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Instrument :
MSVOA_N
ClientSampleId :
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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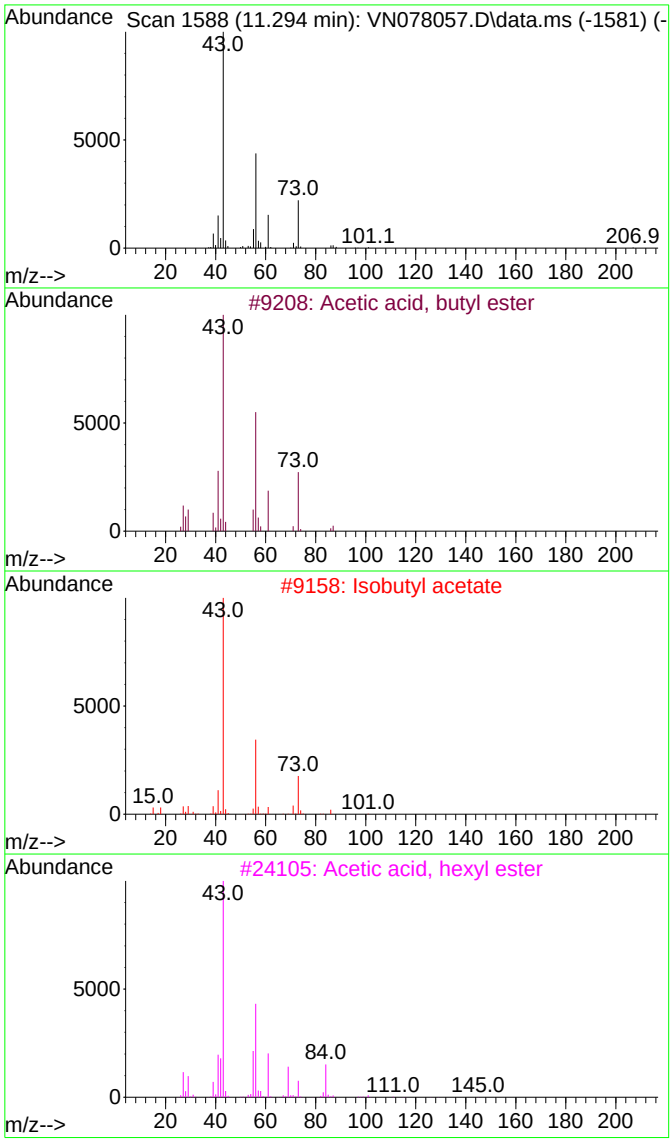
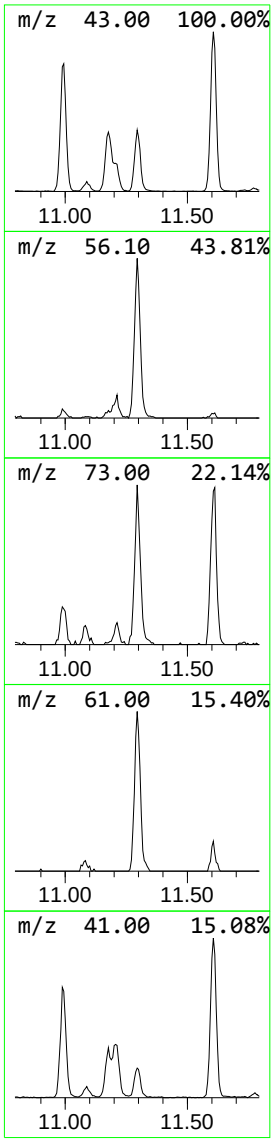
****
Peak Number 8 Acetic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.294	9.32 ug/l	357460	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	Isobutyl acetate	116	C6H12O2	000110-19-0	40
3	Acetic acid, hexyl ester	144	C8H16O2	000142-92-7	36
4	Butane, 1-propoxy-	116	C7H16O	003073-92-5	25
5	Di-n-propyl ether	102	C6H14O	000111-43-3	17





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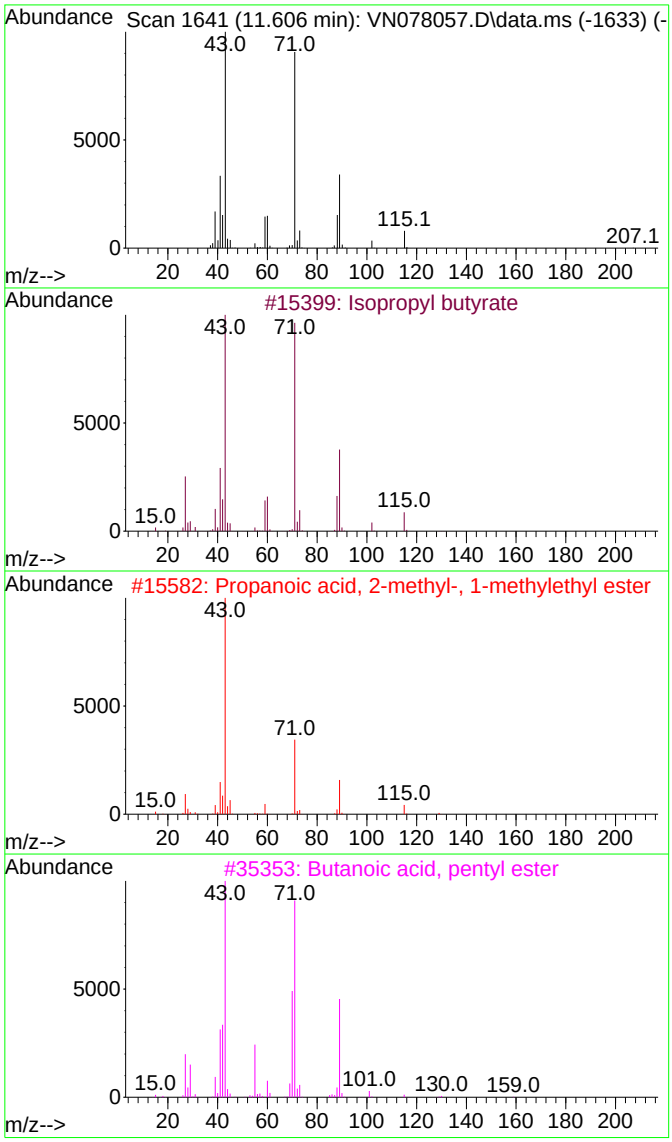
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051523W.M
Quant Title : SW846 8260

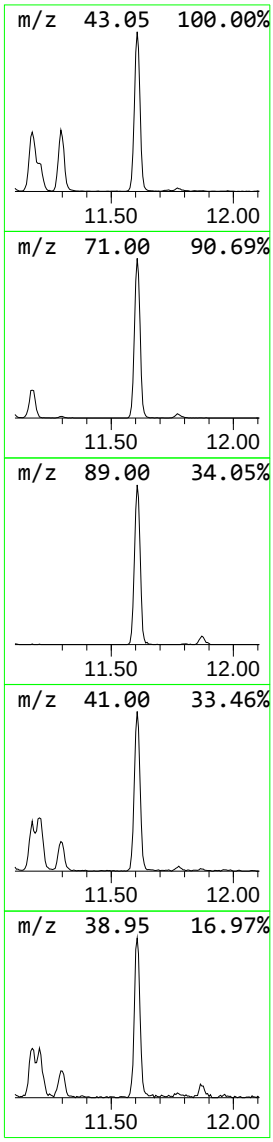
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.606	36.31 ug/l	1393200	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	72
3	Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
4	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	64
5	Ethane-1,1-diol dibutanoate	202	C10H18O4	025572-25-2	59





Tentatively Identified Compound (LSC) summary

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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	5.9	ug/l	189890	2	9.106	1617870	50.0
n-Propyl acetate	9.747	85.9	ug/l	2778780	2	9.106	1617870	50.0
Propanoic acid,...	10.365	20.9	ug/l	675919	2	9.106	1617870	50.0
Isobutyl acetate	10.735	16.6	ug/l	637681	3	11.871	1918390	50.0
Propanoic acid,...	10.994	19.4	ug/l	745808	3	11.871	1918390	50.0
3-Pentanone, 2,...	11.177	7.3	ug/l	279247	3	11.871	1918390	50.0
Propanoic acid,...	11.206	20.6	ug/l	792410	3	11.871	1918390	50.0
Acetic acid, bu...	11.294	9.3	ug/l	357460	3	11.871	1918390	50.0
Isopropyl butyrate	11.606	36.3	ug/l	1393200	3	11.871	1918390	50.0