LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN091619\
Data File : VN058110.D
Acq On : 16 Sep 2019 12:06
Operator : JC/SP
Sample : K4877-06
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : CSA-2-4

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\82N091019W.M
Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.423	194	202	212	rBV4	19447	33205	1.25%	0.169%
2	4.529	841	857	876	rVB4	15996	48867	1.84%	0.249%
3	7.577	1786	1805	1816	rBV2	332797	835470	31.50%	4.258%
4	7.651	1816	1828	1848	rVB	462599	1096331	41.33%	5.588%
5	8.014	1923	1941	1964	rBV	426839	982663	37.05%	5.009%
6	8.153	1969	1984	1997	rBV	82475	207020	7.80%	1.055%
7	8.574	2100	2115	2136	rBV	675716	1422426	53.63%	7.250%
8	9.178	2291	2303	2315	rBV2	35701	75622	2.85%	0.385%
9	9.262	2315	2329	2348	rBV	1419378	2622084	98.85%	13.365%
10	9.898	2514	2527	2543	rBV	234429	405565	15.29%	2.067%
11	10.085	2571	2585	2610	rBV	1433446	2652528	100.00%	13.520%
12	10.281	2636	2646	2659	rVB	53080	87908	3.31%	0.448%
13	10.541	2709	2727	2744	rBV	474246	794649	29.96%	4.050%
14	10.638	2747	2757	2770	rVV3	64373	111322	4.20%	0.567%
15	10.718	2770	2782	2787	rVV	125190	206127	7.77%	1.051%
16	10.763	2787	2796	2815	rVV	548739	909844	34.30%	4.637%
17	10.853	2815	2824	2839	rVB3	28937	52294	1.97%	0.267%
18	11.168	2909	2922	2944	rBV	920227	1470236	55.43%	7.494%
19	11.326	2964	2971	2979	rBV2	19158	27075	1.02%	0.138%
20	11.406	2982	2996	3016	rVV	989873	1729954	65.22%	8.818%
21	11.779	3102	3112	3120	rBV3	21268	39008	1.47%	0.199%
22	11.879	3134	3143	3160	rVB2	89486	157288	5.93%	0.802%
23	12.403	3292	3306	3328	rBV	987744	1666397	62.82%	8.494%
24	13.217	3542	3559	3569	rBV	8507	29327	1.11%	0.149%
25	13.348	3587	3600	3619	rBV	1135828	1869924	70.50%	9.531%
26	15.136	4148	4156	4168	rVB2	17632	28911	1.09%	0.147%
27	16.217	4477	4492	4507	rBV4	26856	57472	2.17%	0.293%

Sum of corrected areas: 19619517

LSC Report - Integrated Chromatogram

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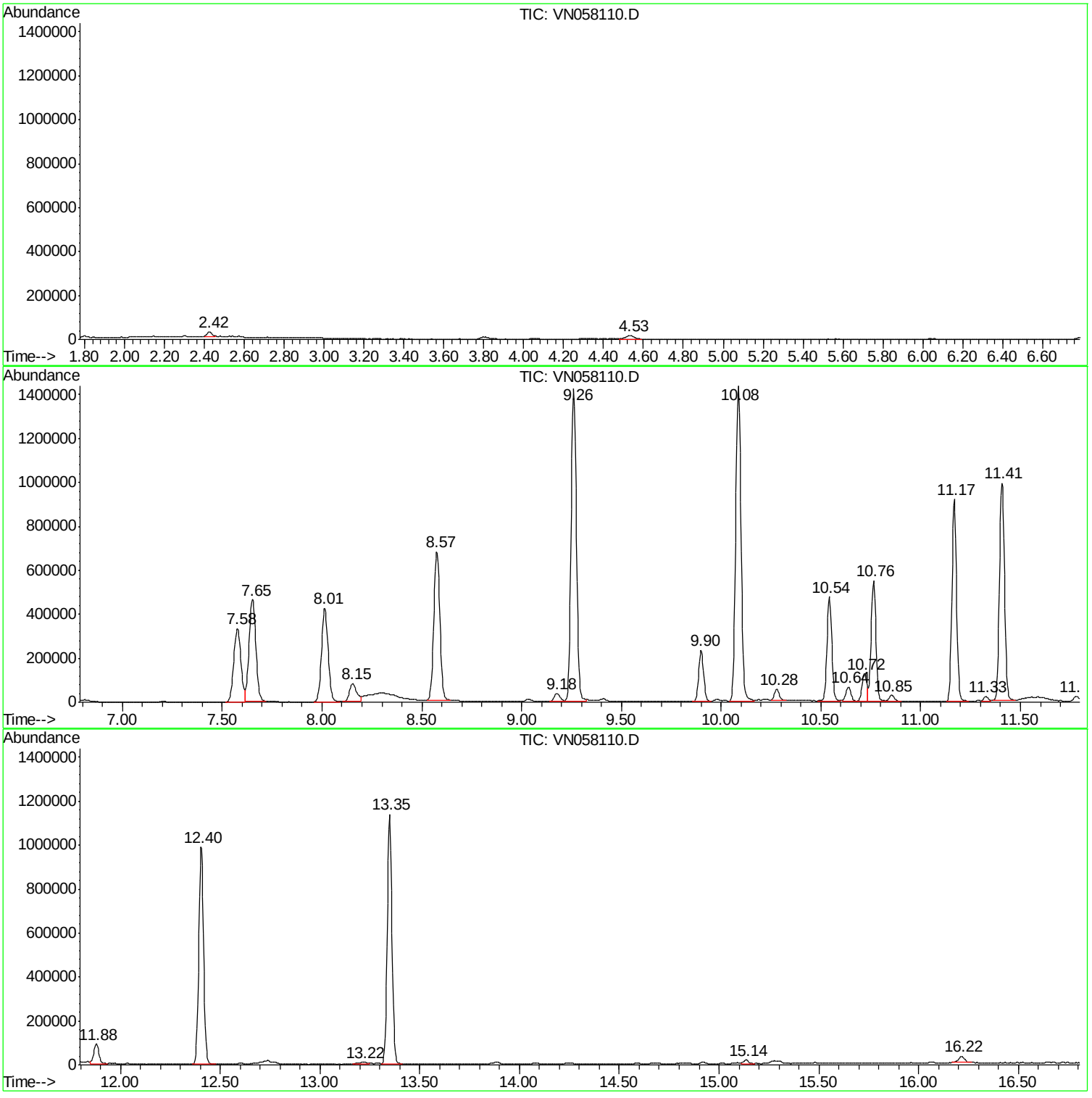
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : CSA-2-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091019W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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Quant Title : SW846 8260

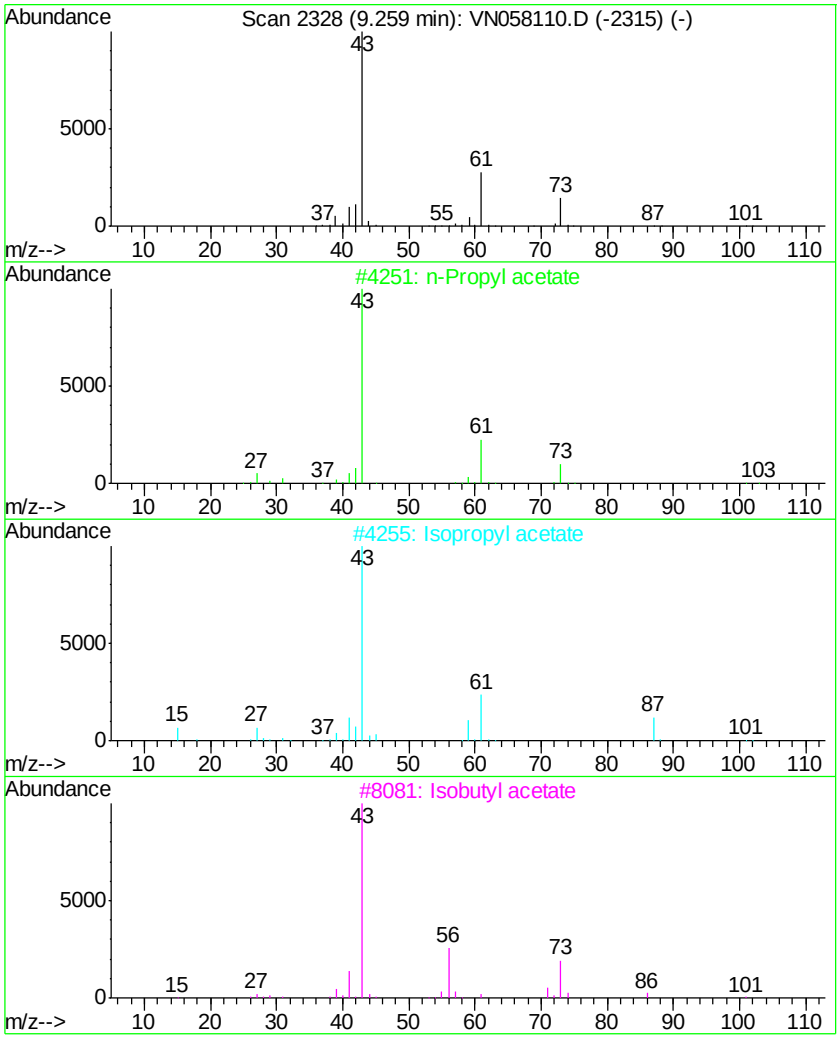
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

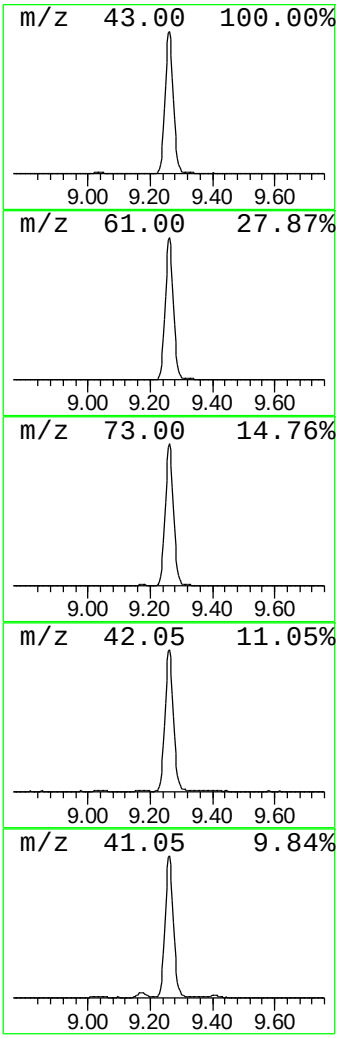
****

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.26	92.17 ug/l	2622080	1,4-Difluorobenzene	8.57

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	36
3	Isobutyl acetate	116	C6H12O2	000110-19-0	9
4	Isobutylamine	73	C4H11N	000078-81-9	7
5	1-Butanamine	73	C4H11N	000109-73-9	5





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Operator : JC/SP
Sample : K4877-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : CSA-2-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091019W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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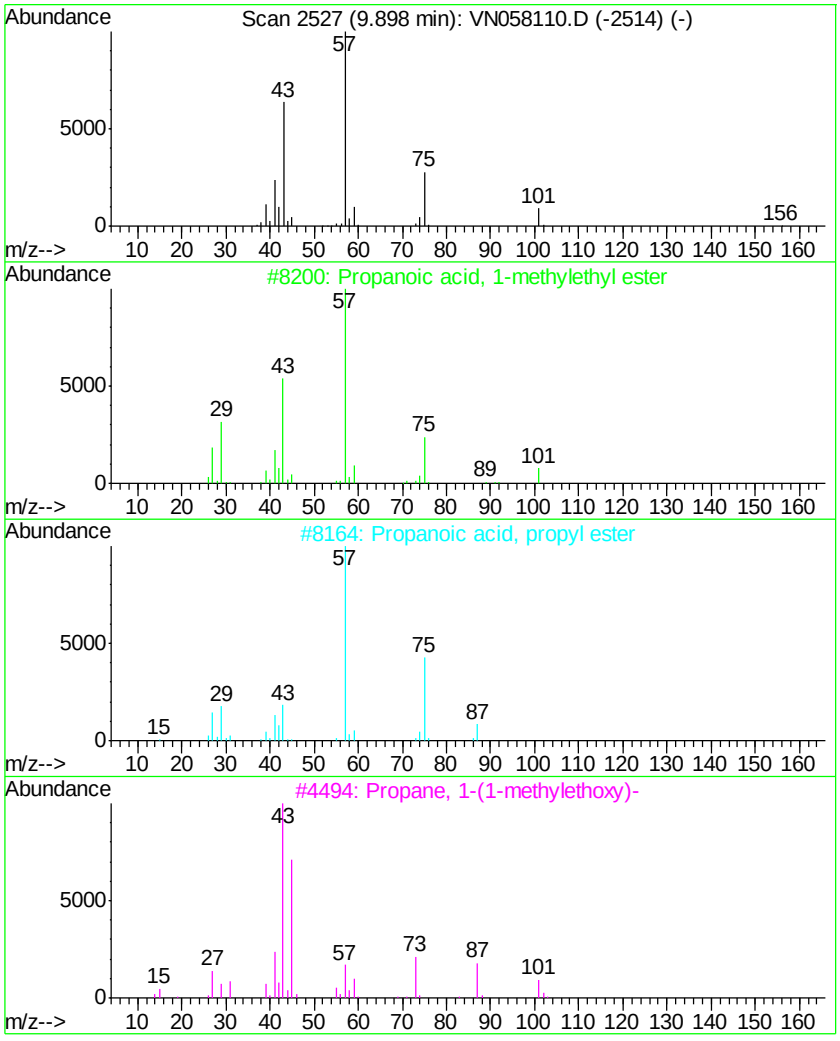
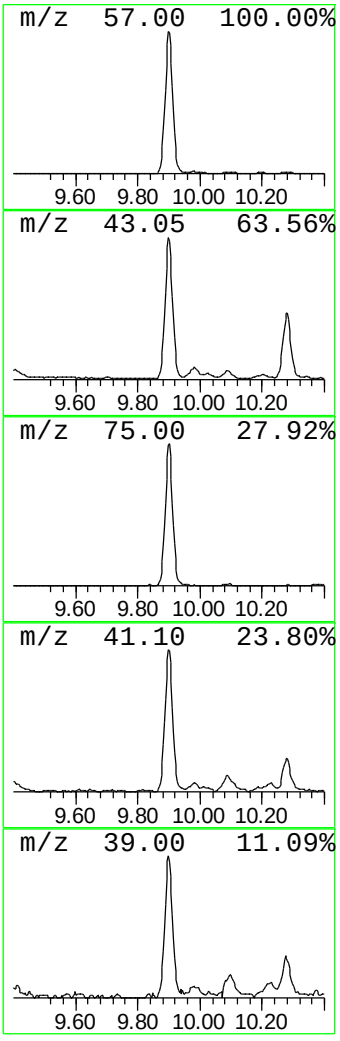
Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.90	14.26 ug/l	405565	1,4-Difluorobenzene	8.57

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	45
3	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	25
4	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	14
5	Azetidine	57	C3H7N	000503-29-7	12





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Operator : JC/SP
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Instrument : MSVOA_N
ClientSampleId : CSA-2-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091019W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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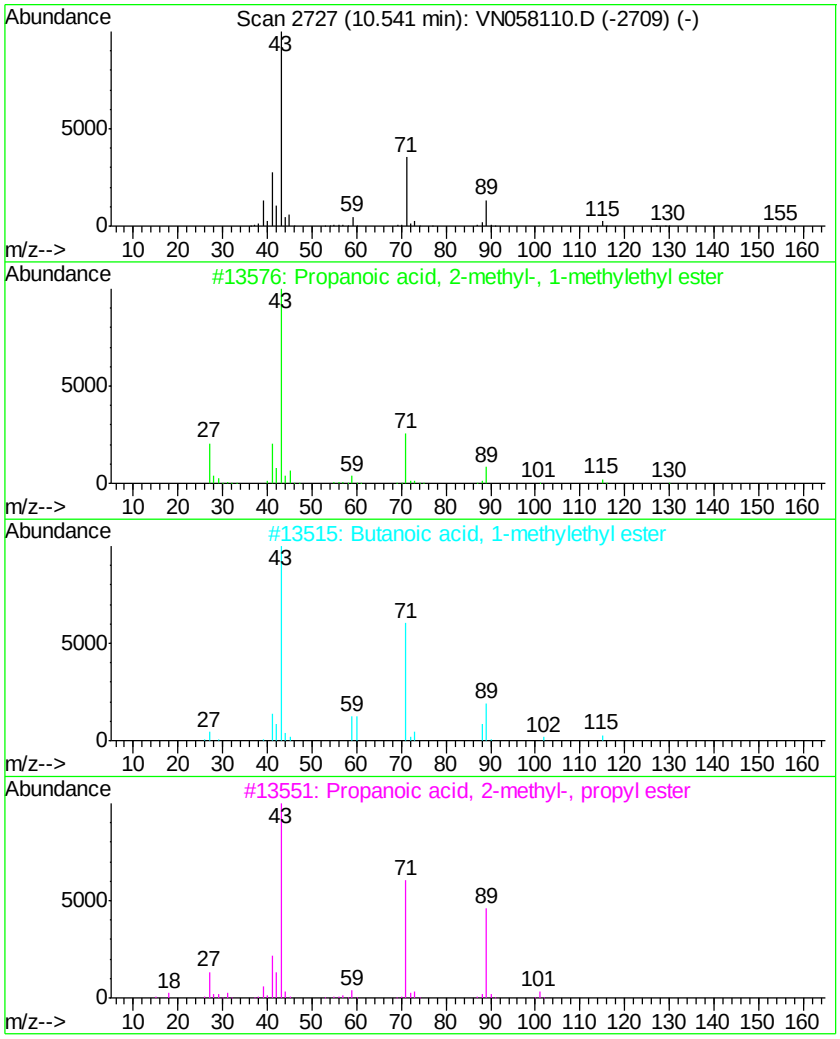
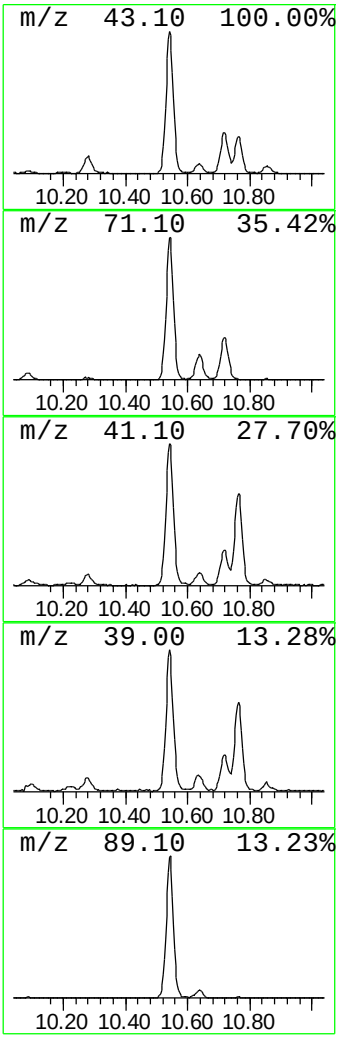
****
Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.54	22.97 ug/l	794649	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	72
3	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
4	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50
5	Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	42





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Instrument : MSVOA_N
ClientSampleId : CSA-2-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091019W.M
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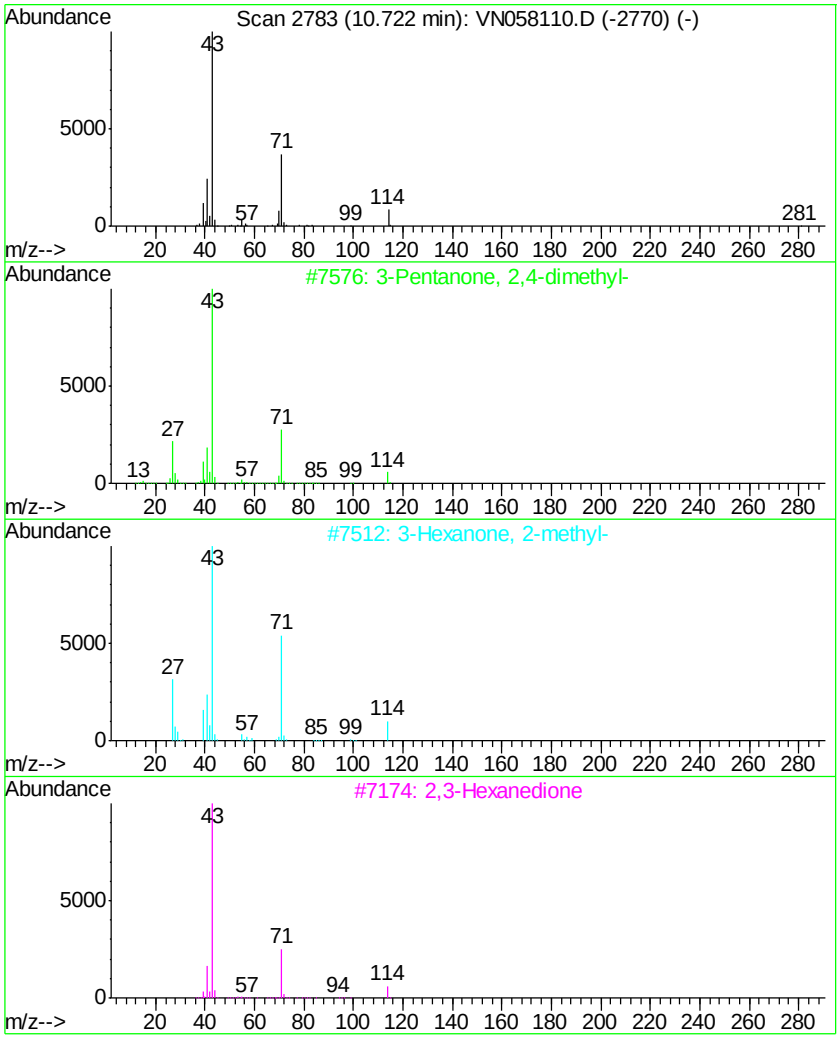
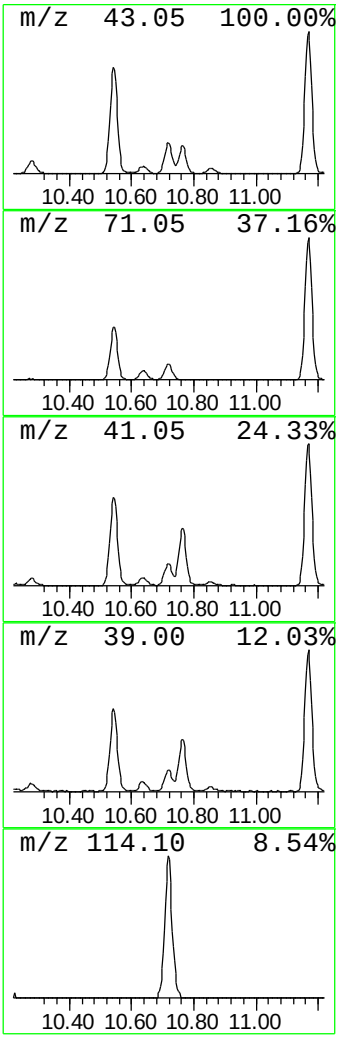
Peak Number 4 3-Pentanone, 2,4-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.72	5.96 ug/l	206127	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	80
2	3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	59
3	2,3-Hexanedione	114	C6H10O2	003848-24-6	59
4	Pyrrolidine	71	C4H9N	000123-75-1	47
5	2,5-Hexanedione	114	C6H10O2	000110-13-4	40





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ALS Vial : 10 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : CSA-2-4

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N091019W.M
Quant Title : SW846 8260

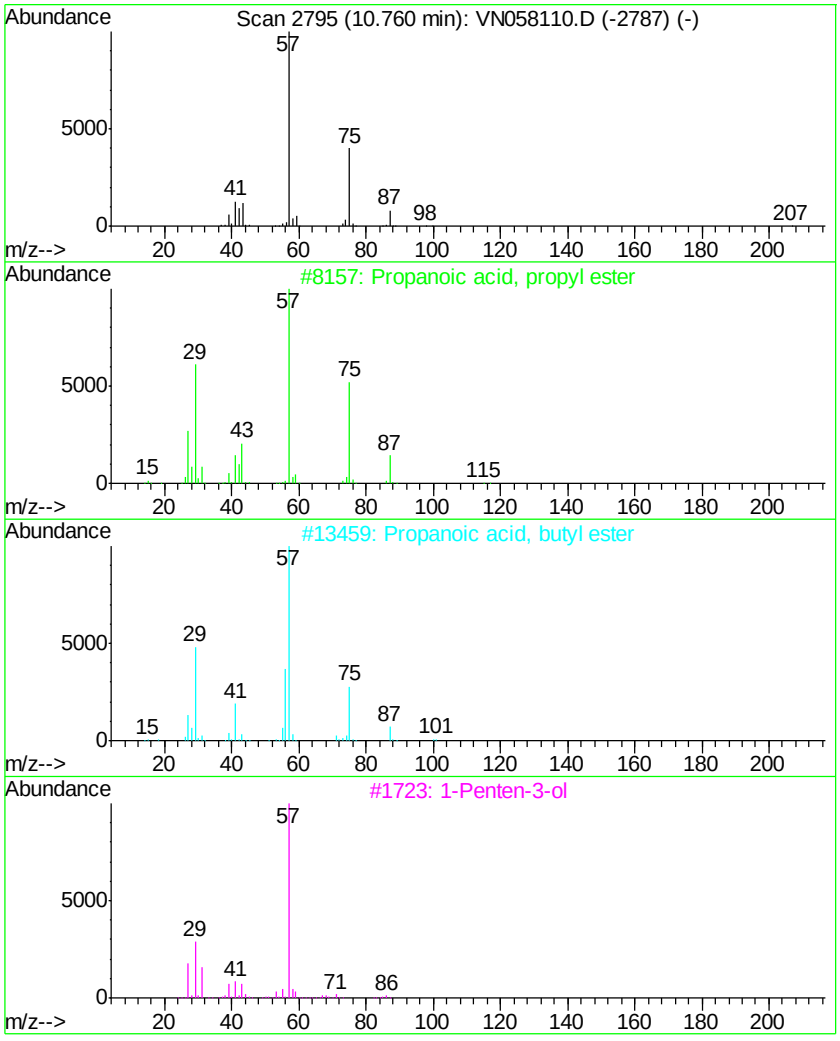
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

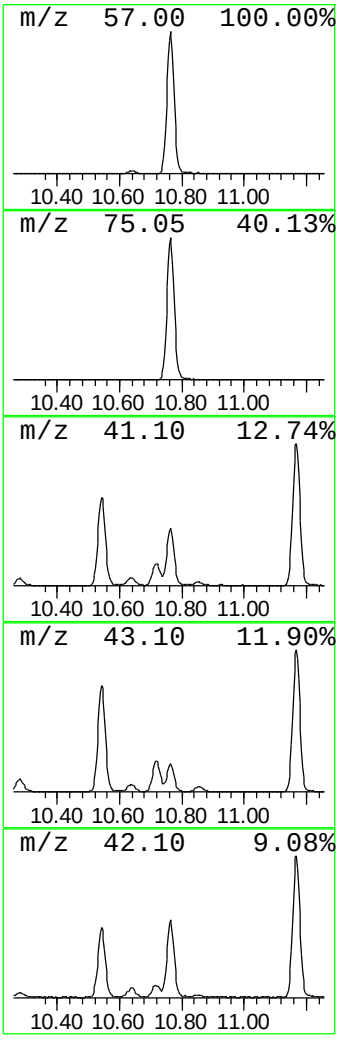
****

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.76	26.30 ug/l	909844	Chlorobenzene-d5	11.41

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	25
3	1-Penten-3-ol	86	C5H10O	000616-25-1	9
4	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	9
5	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9





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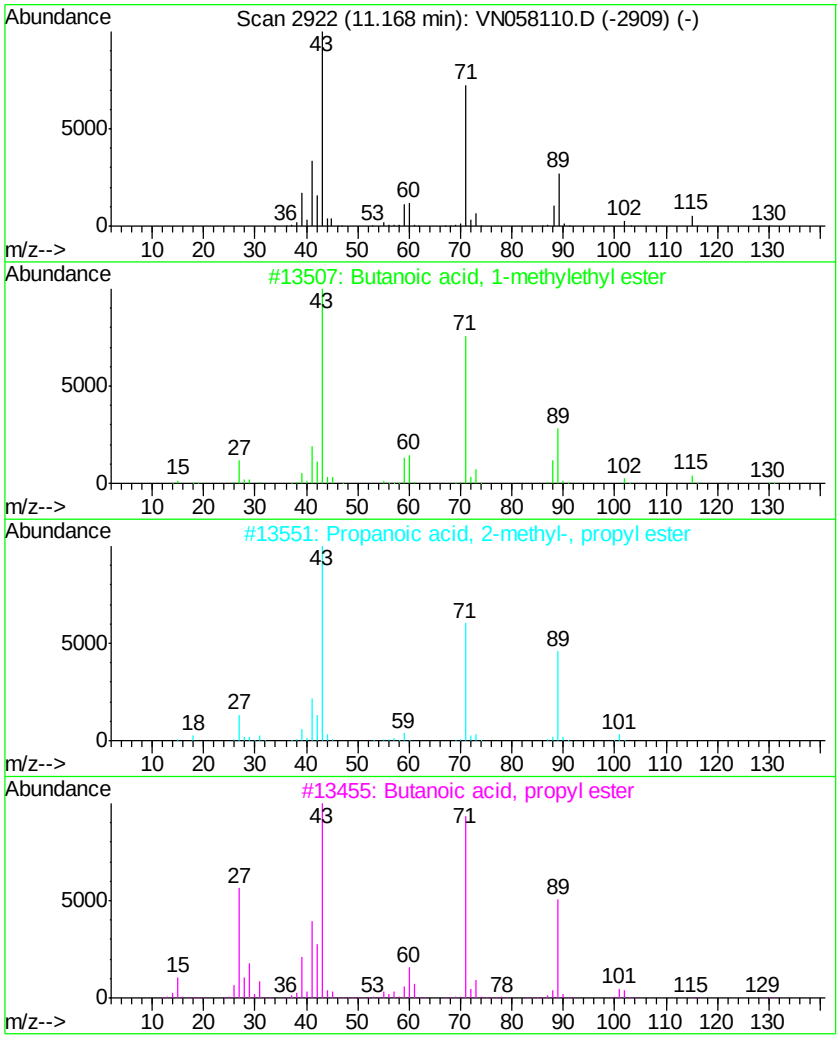
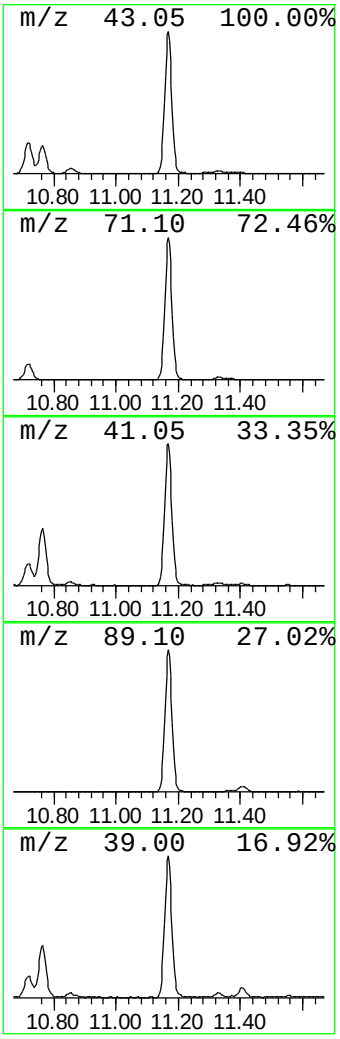
****

Peak Number 6 Butanoic acid, 1-methylethy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.17	42.49 ug/l	1470240	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
2	Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	59
3	Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
4	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	50
5	Ethane-1,1-diol dibutanoate	202	C10H18O4	025572-25-2	50





Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Propyl acetate	9.26	92.2	ug/l	2622080	2	8.57	1422430	50.0
Propanoic acid, 1...	9.90	14.3	ug/l	405565	2	8.57	1422430	50.0
Propanoic acid, 2...	10.54	23.0	ug/l	794649	3	11.41	1729950	50.0
3-Pentanone, 2,4-...	10.72	6.0	ug/l	206127	3	11.41	1729950	50.0
Propanoic acid, p...	10.76	26.3	ug/l	909844	3	11.41	1729950	50.0
Butanoic acid, 1-...	11.17	42.5	ug/l	1470240	3	11.41	1729950	50.0