LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN090420\
Data File : VN063254.D
Acq On : 4 Sep 2020 17:48
Operator : JC/MD
Sample : L3866-01
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TOTE-31230

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\82N083120W.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	2.139	114	124	131	rBV4	14275	24363	1.24%	0.157%
2	2.422	201	212	223	rBV2	46536	91599	4.65%	0.591%
3	3.779	619	634	655	rBV2	33549	90153	4.58%	0.582%
4	4.505	848	860	882	rVB5	21875	68777	3.49%	0.444%
5	5.361	1108	1126	1128	rBV5	24494	53035	2.69%	0.342%
6	6.499	1462	1480	1496	rBV4	40171	127614	6.48%	0.824%
7	6.791	1551	1571	1590	rBV3	28121	91788	4.66%	0.593%
8	7.550	1789	1807	1819	rBV3	230588	579753	29.46%	3.743%
9	7.627	1819	1831	1848	rVB2	354977	847412	43.05%	5.472%
10	7.987	1923	1943	1966	rBV	292148	735721	37.38%	4.750%
11	8.129	1973	1987	2002	rVB2	40618	88827	4.51%	0.574%
12	8.251	2002	2025	2034	rBV7	62342	214559	10.90%	1.385%
13	8.412	2066	2075	2094	rVB4	55085	139311	7.08%	0.900%
14	8.550	2102	2118	2132	rBV	628615	1302738	66.19%	8.412%
15	8.634	2133	2144	2160	rVB2	282843	588387	29.89%	3.799%
16	9.007	2246	2260	2273	rBV2	77117	157403	8.00%	1.016%
17	9.135	2284	2300	2317	rBV3	124534	286372	14.55%	1.849%
18	9.238	2318	2332	2352	rVV	758797	1415142	71.90%	9.137%
19	9.393	2369	2380	2390	rVB4	27697	57906	2.94%	0.374%
20	9.875	2518	2530	2542	rBV2	48798	88392	4.49%	0.571%
21	9.955	2542	2555	2566	rBV3	27159	52040	2.64%	0.336%
22	10.061	2573	2588	2600	rBV	1058076	1968241	100.00%	12.709%
23	10.126	2600	2608	2629	rVB	172280	322458	16.38%	2.082%
24	10.238	2634	2643	2644	rBV6	18334	21730	1.10%	0.140%
25	10.328	2664	2671	2677	rBV3	27018	47435	2.41%	0.306%
26	10.508	2715	2727	2740	rBV6	43789	109193	5.55%	0.705%
27	10.611	2751	2759	2770	rVB3	29584	50512	2.57%	0.326%
28	10.692	2775	2784	2785	rBV2	16996	20298	1.03%	0.131%
29	10.737	2787	2798	2815	rVB3	137195	268998	13.67%	1.737%
30	10.827	2815	2826	2840	rBV	121839	214850	10.92%	1.387%
31	11.113	2903	2915	2920	rBV2	66111	116863	5.94%	0.755%
32	11.380	2981	2998	3013	rBV	1019139	1781105	90.49%	11.500%
33	11.531	3038	3045	3063	rVB5	33414	65526	3.33%	0.423%
34	11.634	3063	3077	3088	rVB7	25742	57404	2.92%	0.371%

LSC Area Percent Report

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Operator : JC/MD
Sample : L3866-01
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TOTE-31230

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\82N083120W.M
Title : SW846 8260

35	11.704	3089	3099	3109	rBV7	13180	27019	1.37%	0.174%
36	11.859	3135	3147	3163	rVB8	18530	33129	1.68%	0.214%
37	12.007	3185	3193	3206	rVB	30606	53385	2.71%	0.345%
38	12.106	3212	3224	3240	rBV3	61212	117495	5.97%	0.759%
39	12.380	3295	3309	3335	rVB	754144	1299450	66.02%	8.390%
40	12.708	3404	3411	3421	rVB4	24855	40956	2.08%	0.264%
41	12.778	3426	3433	3441	rVB8	17076	29381	1.49%	0.190%
42	13.100	3528	3533	3544	rVB5	23140	36812	1.87%	0.238%
43	13.171	3548	3555	3564	rBV9	18119	25229	1.28%	0.163%
44	13.318	3587	3601	3624	rBV	928877	1570453	79.79%	10.140%
45	13.428	3626	3635	3645	rBV2	42714	73108	3.71%	0.472%
46	13.492	3647	3655	3663	rBV8	16292	35072	1.78%	0.226%

Sum of corrected areas: 15487394

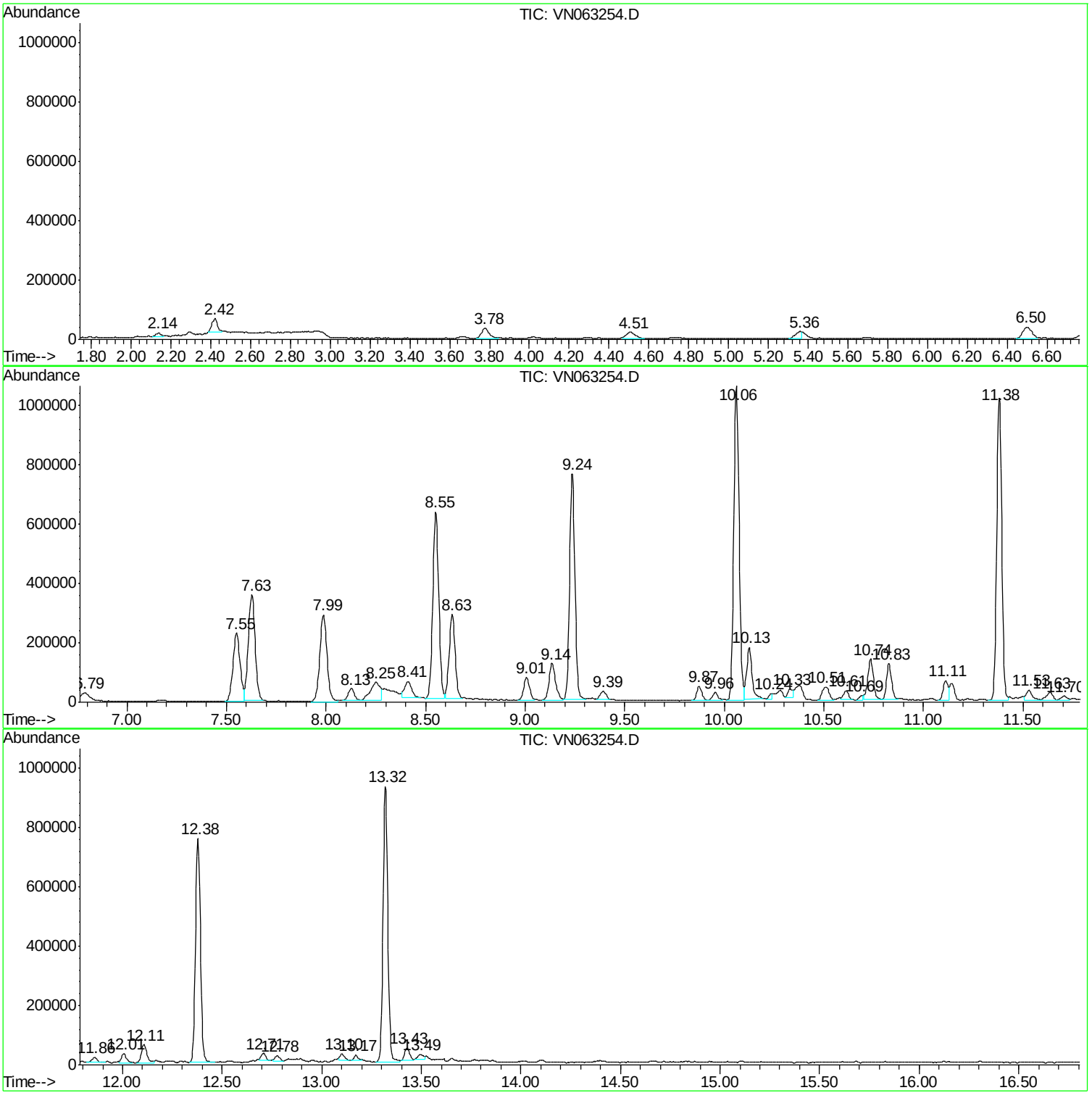
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN090420\
Data File : VN063254.D
Acq On : 4 Sep 2020 17:48
Operator : JC/MD
Sample : L3866-01
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TOTE-31230

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N083120W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090420\
Data File : VN063254.D
Acq On : 4 Sep 2020 17:48
Operator : JC/MD
Sample : L3866-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TOTE-31230

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N083120W.M
Quant Title : SW846 8260

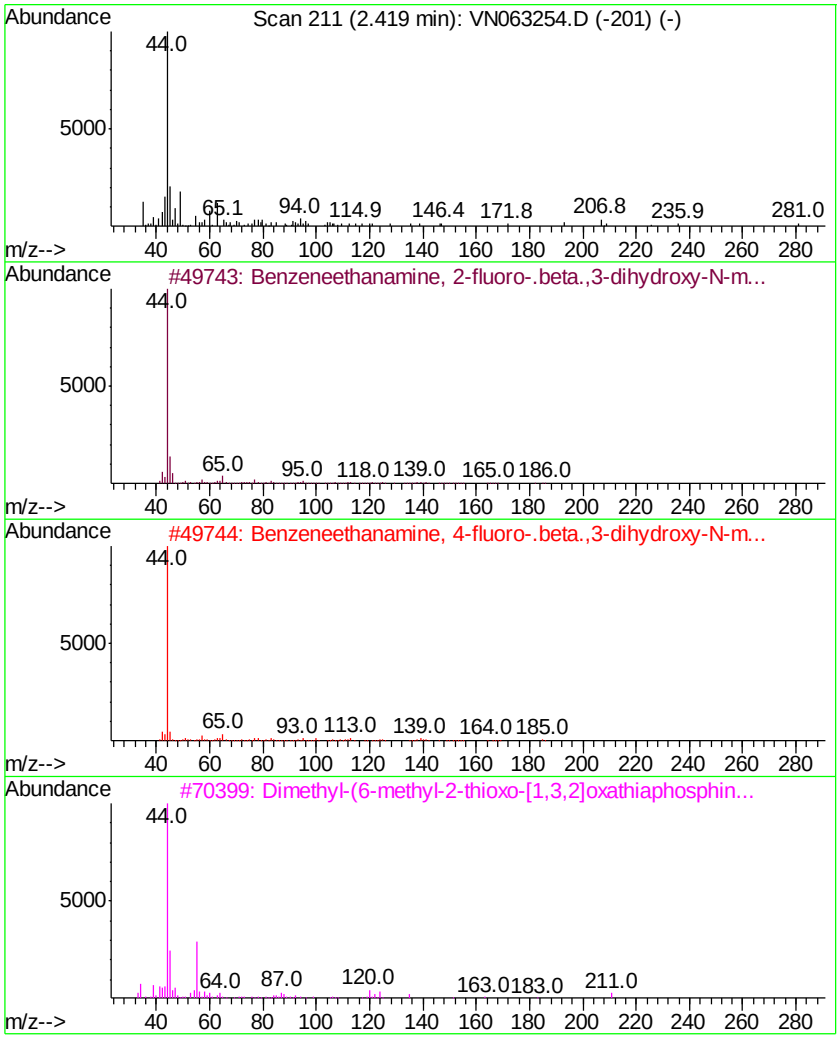
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

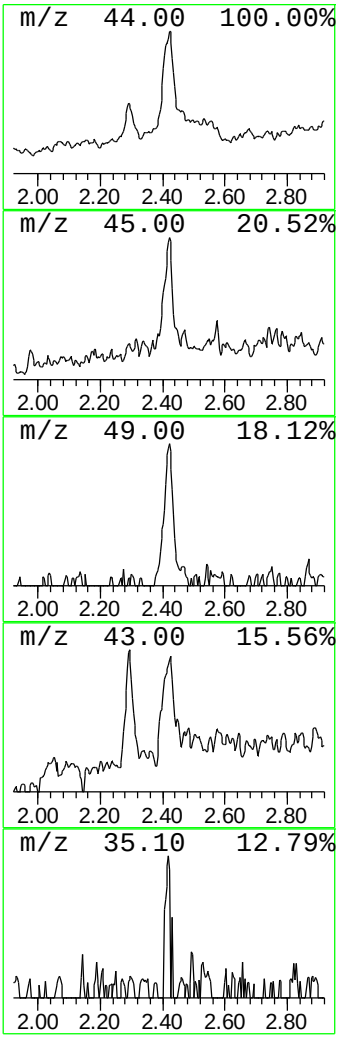
****

Peak Number 1 Benzeneethanamine, 2-fluoro... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.42	5.40 ug/l	91599	Pentafluorobenzene	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzeneethanamine, 2-fluoro-.bet...	185	C9H12FNO2	103439-04-9	53
2	Benzeneethanamine, 4-fluoro-.bet...	185	C9H12FNO2	103439-06-1	50
3	Dimethyl-(6-methyl-2-thioxo-[1,3...	211	C6H14NOPS2	139575-19-2	50
4	Phenylephrine	167	C9H13NO2	000059-42-7	50
5	Phenethylamine, p,.alpha.-dimethyl-	149	C10H15N	000064-11-9	47





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090420\
Data File : VN063254.D
Acq On : 4 Sep 2020 17:48
Operator : JC/MD
Sample : L3866-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TOTE-31230

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N083120W.M
Quant Title : SW846 8260

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

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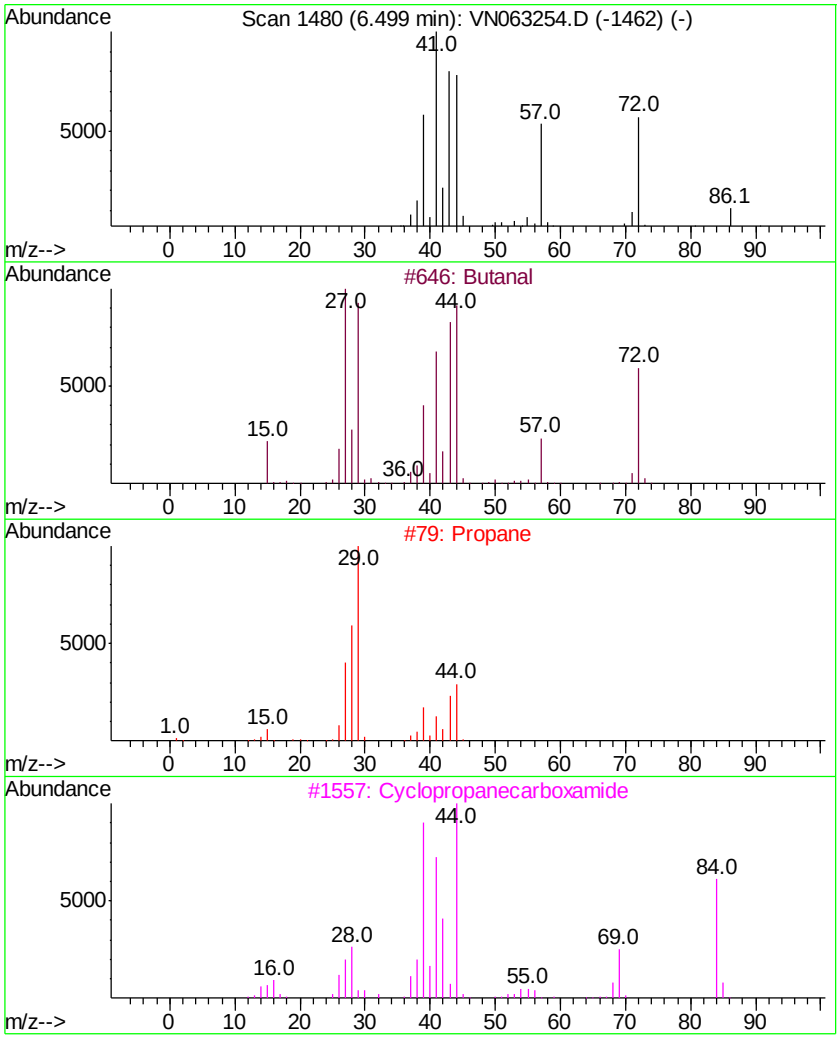
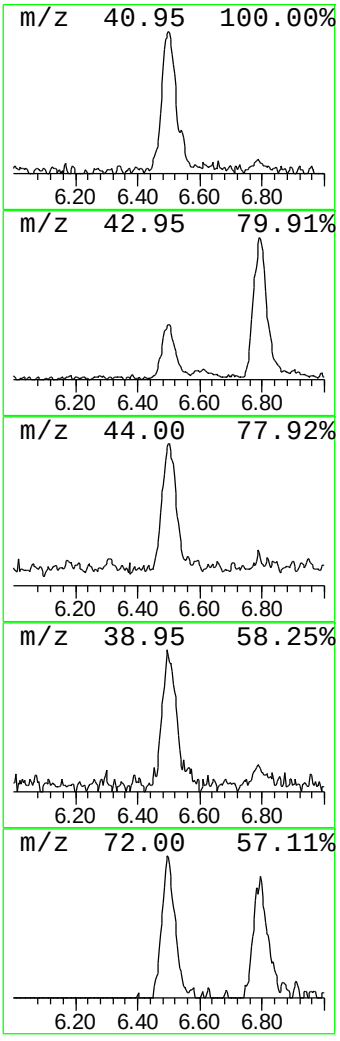
Peak Number 2 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	7.53 ug/l	127614	Pentafluorobenzene	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	58
2	Propane	44	C3H8	000074-98-6	50
3	Cyclopropanecarboxamide	85	C4H7NO	006228-73-5	38
4	Butanal, 3-methyl-	86	C5H10O	000590-86-3	37
5	2-Hexynoic acid	112	C6H8O2	000764-33-0	32





Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN090420\
Data File : VN063254.D
Acq On : 4 Sep 2020 17:48
Operator : JC/MD
Sample : L3866-01
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TOTE-31230

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N083120W.M
Quant Title : SW846 8260

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

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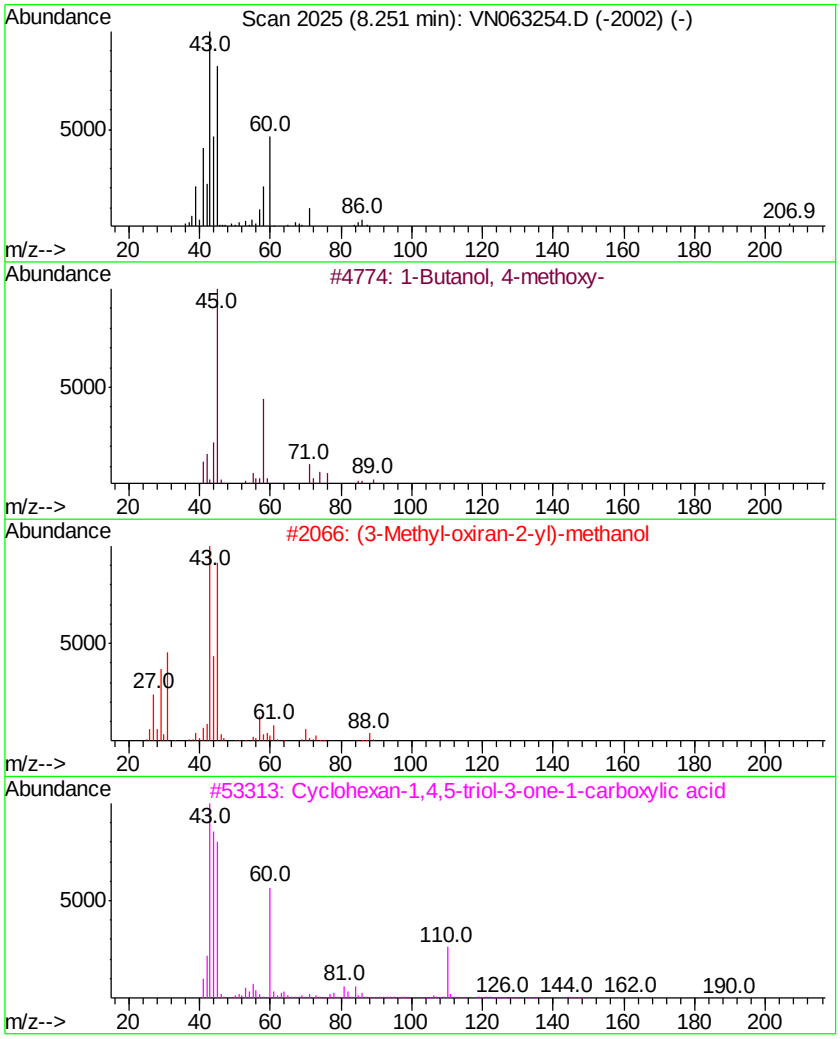
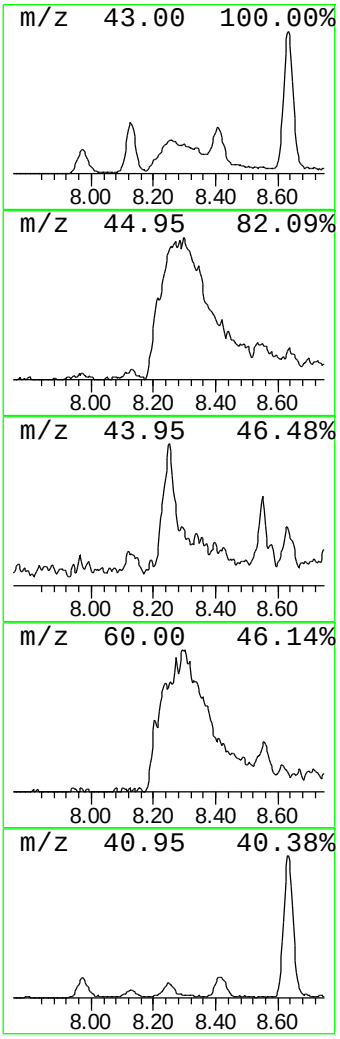
Peak Number 3 unknown8.25 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.25	8.23 ug/l	214559	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol, 4-methoxy-	104	C5H12O2	000111-32-0	47
2	(3-Methyl-oxiran-2-yl)-methanol	88	C4H8O2	1000194-22-9	43
3	Cyclohexan-1,4,5-triol-3-one-1-c...	190	C7H10O6	1000128-45-5	38
4	Propanoic acid, 2-(aminooxy)-	105	C3H7NO3	002786-22-3	38
5	Acetic acid	60	C2H4O2	000064-19-7	38





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090420\
Data File : VN063254.D
Acq On : 4 Sep 2020 17:48
Operator : JC/MD
Sample : L3866-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TOTE-31230

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N083120W.M
Quant Title : SW846 8260

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

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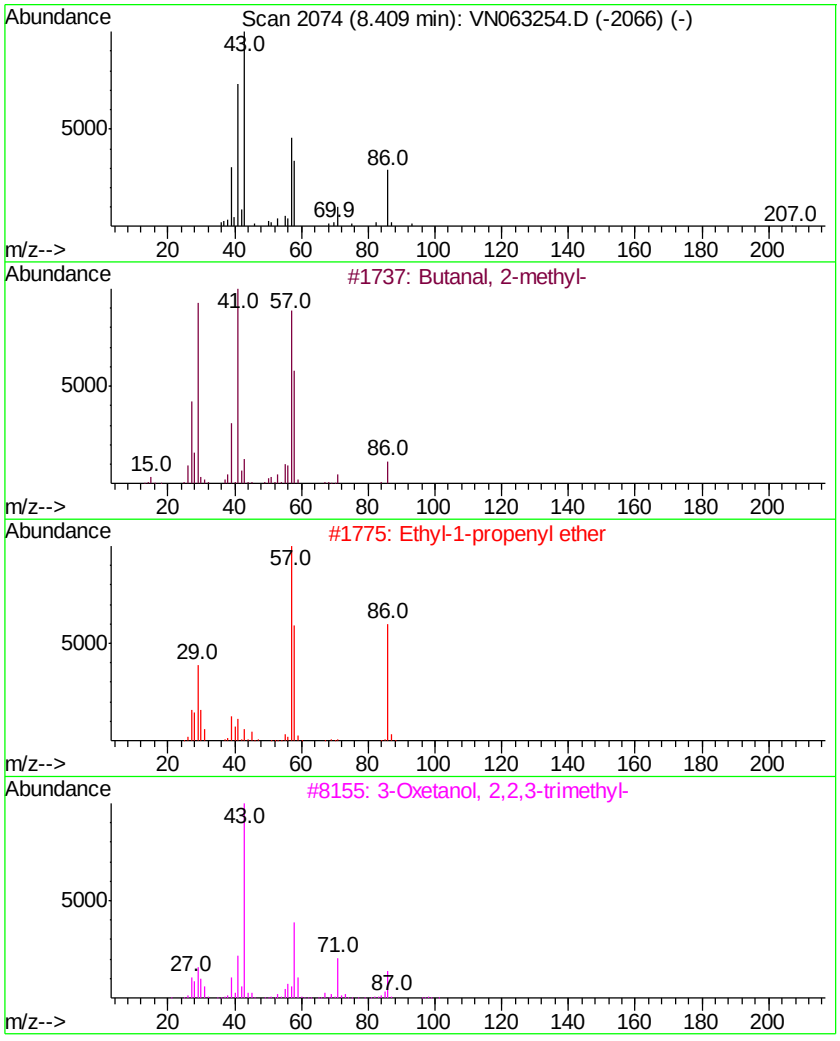
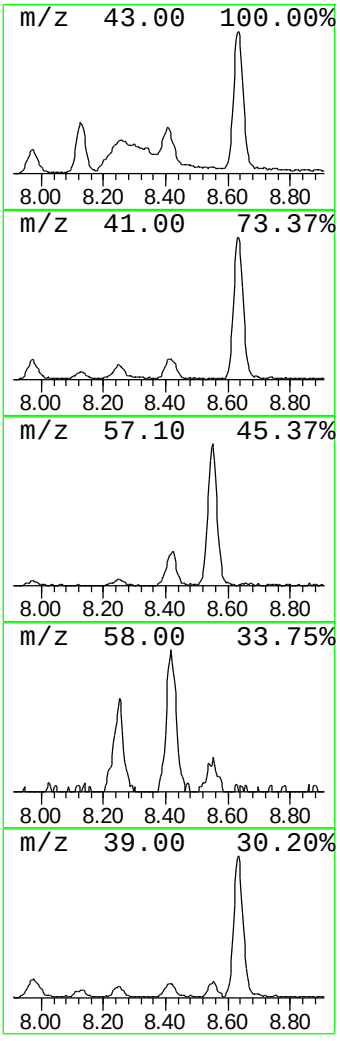
Peak Number 4 unknown8.41 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	5.35 ug/l	139311	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal, 2-methyl-	86	C5H10O	000096-17-3	47
2	Ethyl-1-propenyl ether	86	C5H10O	000928-55-2	37
3	3-Oxetanol, 2,2,3-trimethyl-	116	C6H12O2	025910-96-7	28
4	2-Propenoic acid, 2-methyl-	86	C4H6O2	000079-41-4	27
5	Oxalic acid, allyl pentyl ester	200	C10H16O4	1000309-23-2	27





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090420\
Data File : VN063254.D
Acq On : 4 Sep 2020 17:48
Operator : JC/MD
Sample : L3866-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TOTE-31230

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N083120W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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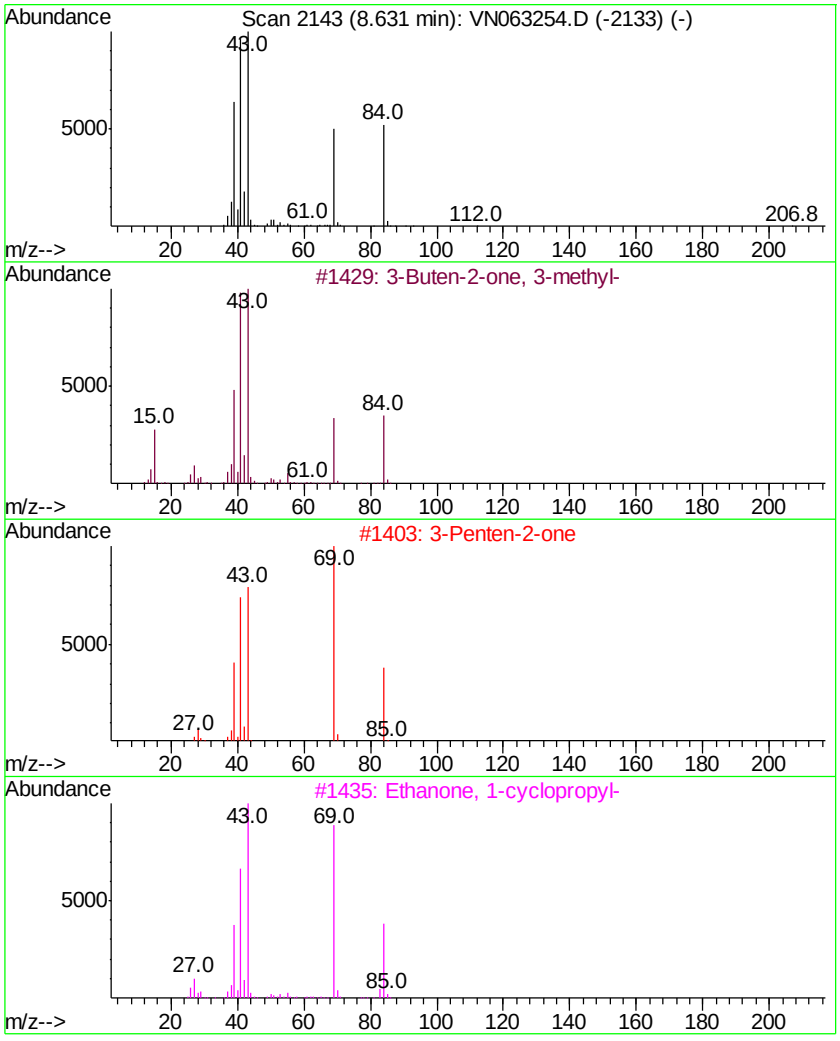
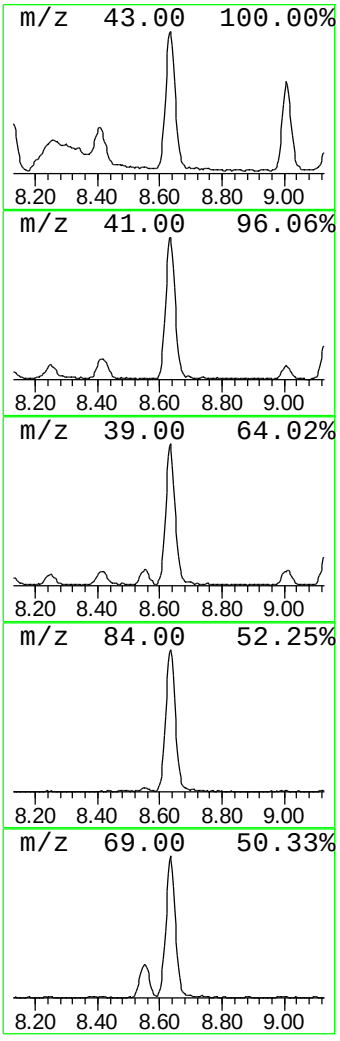
****

Peak Number 5 3-Buten-2-one, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.63	22.58 ug/l	588387	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	90
2	3-Penten-2-one	84	C5H8O	000625-33-2	83
3	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	49
4	Dicyclopropyl carbinol	112	C7H12O	014300-33-5	45
5	3-Penten-2-one, (E)-	84	C5H8O	003102-33-8	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN090420\
Data File : VN063254.D
Acq On : 4 Sep 2020 17:48
Operator : JC/MD
Sample : L3866-01
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TOTE-31230

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N083120W.M
Quant Title : SW846 8260

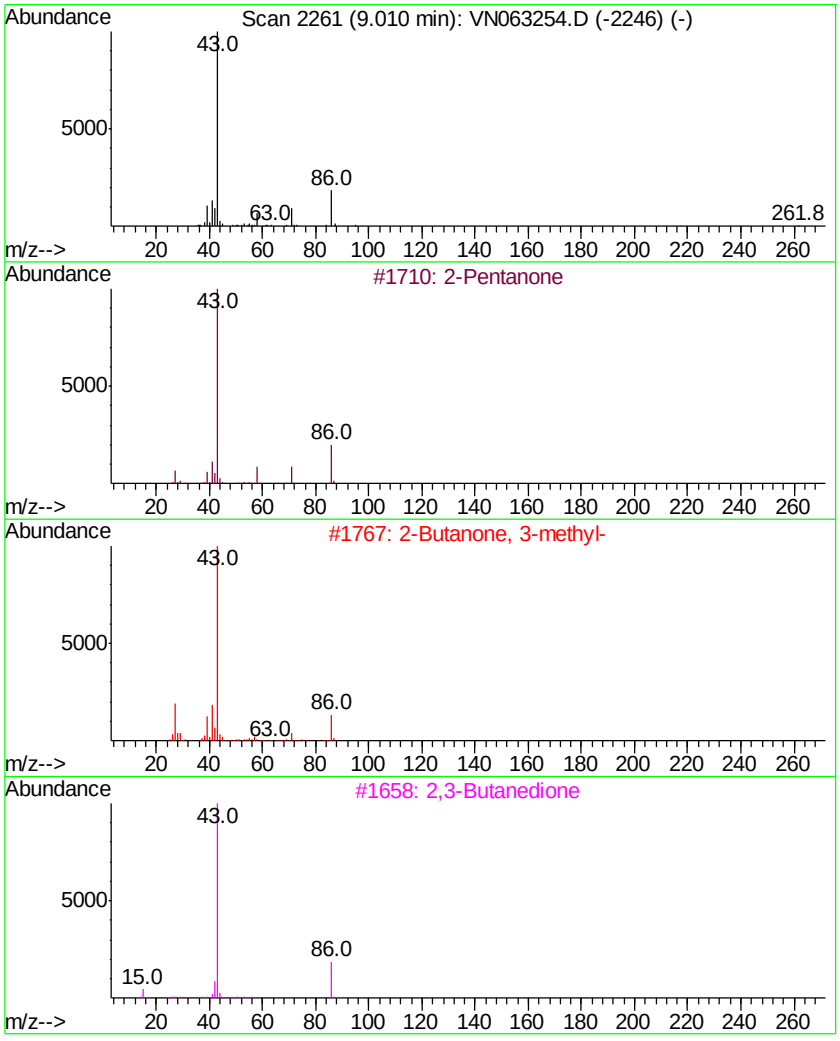
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

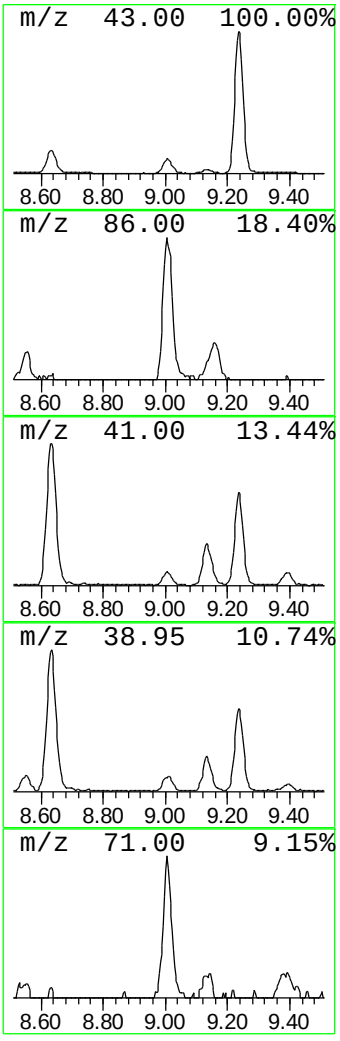
****

Peak Number 6 2-Pentanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.01	6.04 ug/l	157403	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	72
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	64
3	2,3-Butanedione	86	C4H6O2	000431-03-8	38
4	Isobutane	58	C4H10	000075-28-5	16
5	2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN090420\
Data File : VN063254.D
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Operator : JC/MD
Sample : L3866-01
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TOTE-31230

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N083120W.M
Quant Title : SW846 8260

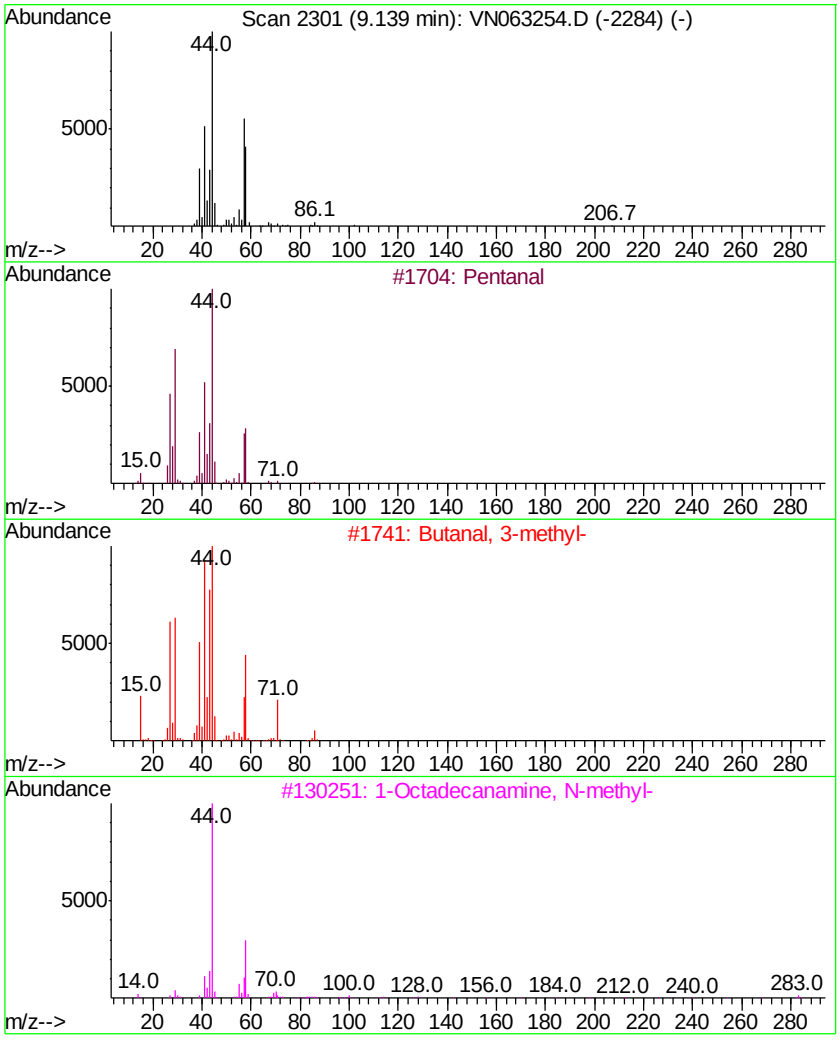
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

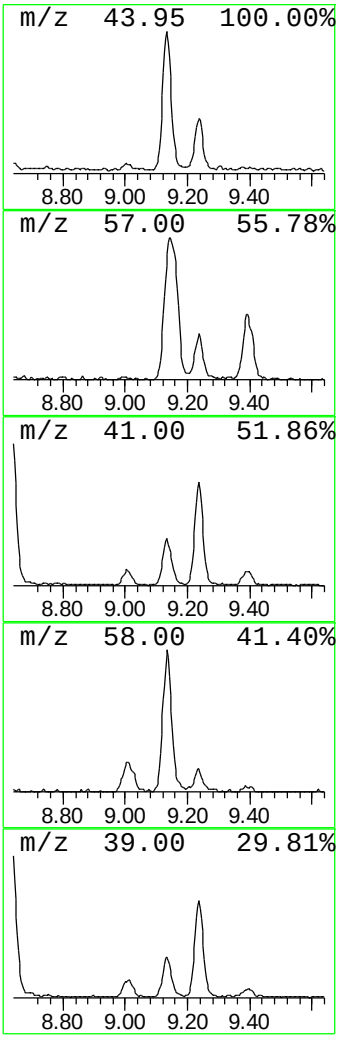
****

Peak Number 7 Pentanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.14	10.99 ug/l	286372	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	86
2	Butanal, 3-methyl-	86	C5H10O	000590-86-3	53
3	1-Octadecanamine, N-methyl-	283	C19H41N	002439-55-6	40
4	Cyclopropyl carbinol	72	C4H8O	002516-33-8	33
5	Carbonic acid, ethyl 2-propenyl ...	130	C6H10O3	001469-70-1	12





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN090420\
Data File : VN063254.D
Acq On : 4 Sep 2020 17:48
Operator : JC/MD
Sample : L3866-01
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TOTE-31230

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N083120W.M
Quant Title : SW846 8260

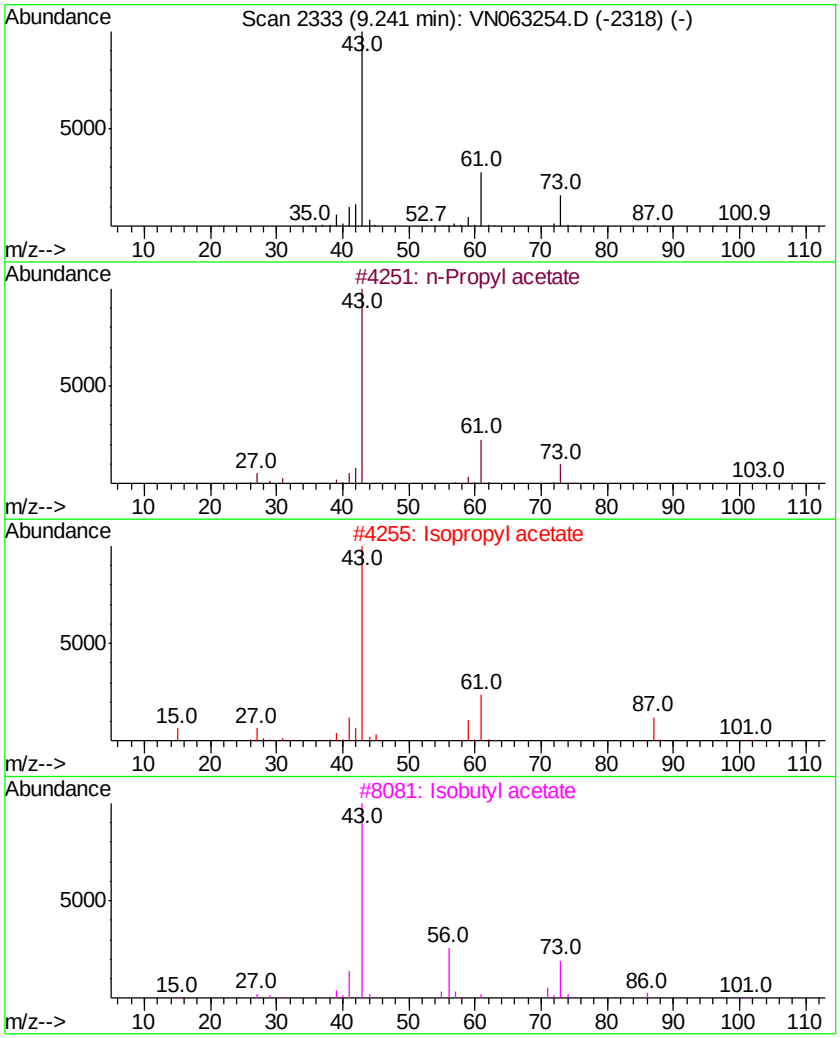
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

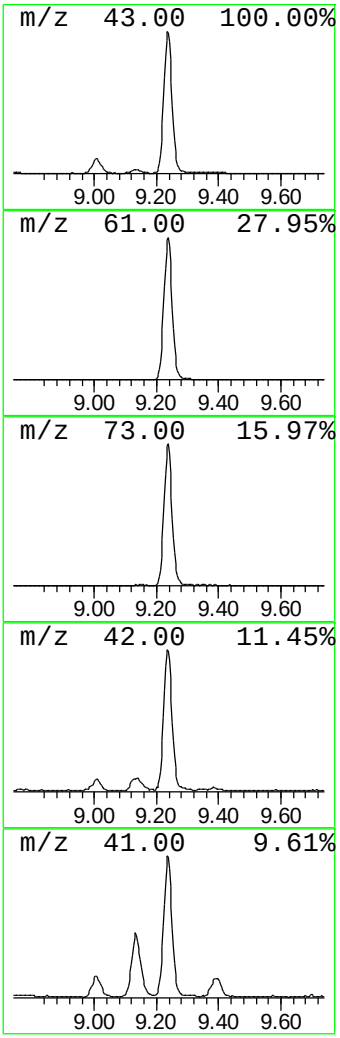
****

Peak Number 8 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.24	54.31 ug/l	1415140	1,4-Difluorobenzene	8.55

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	1-Butanamine	73	C4H11N	000109-73-9	7
5	Isobutylamine	73	C4H11N	000078-81-9	7





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090420\
Data File : VN063254.D
Acq On : 4 Sep 2020 17:48
Operator : JC/MD
Sample : L3866-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TOTE-31230

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N083120W.M
Quant Title : SW846 8260

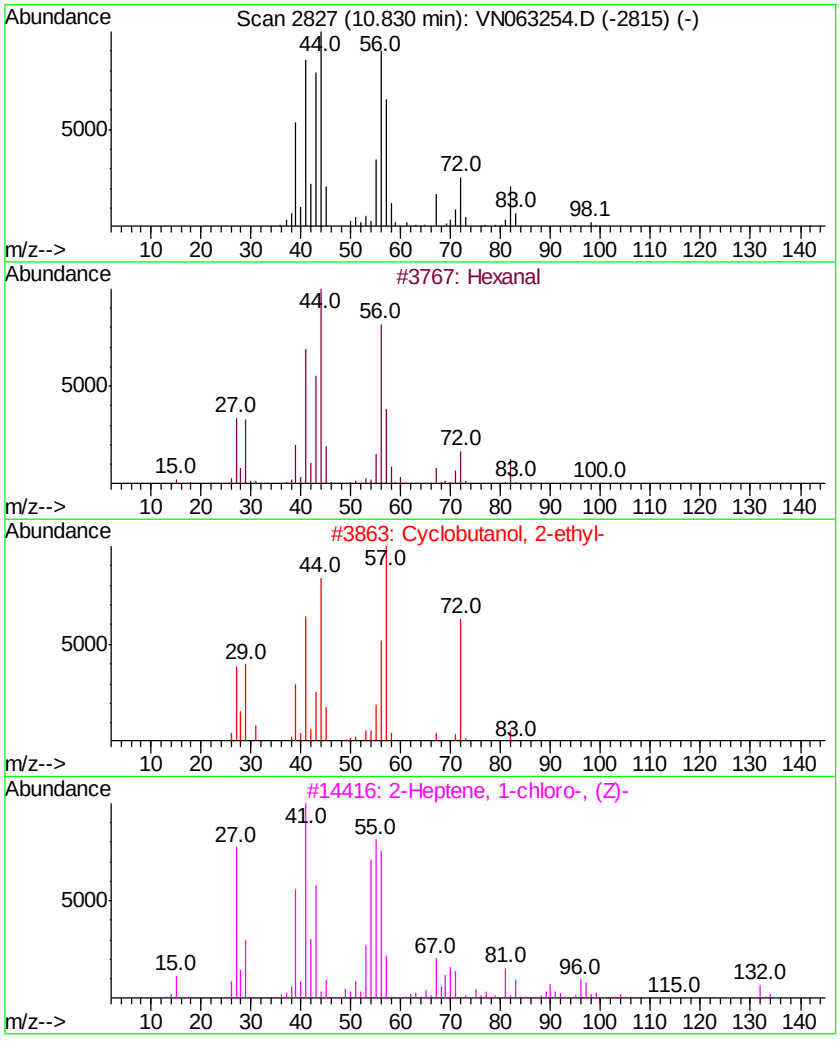
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

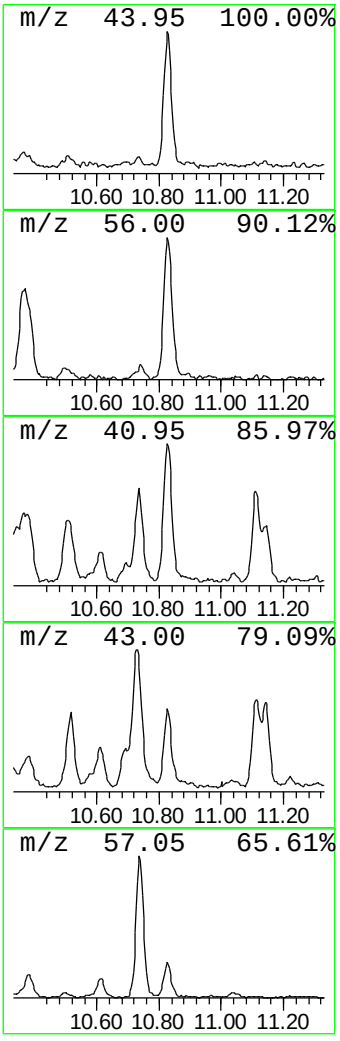
****

Peak Number 9 Hexanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.83	6.03 ug/l	214850	Chlorobenzene-d5	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	59
2	Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	50
3	2-Heptene, 1-chloro-, (Z)-	132	C7H13Cl	055638-53-4	38
4	Butanal	72	C4H8O	000123-72-8	30
5	1-Butene	56	C4H8	000106-98-9	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN090420\
Data File : VN063254.D
Acq On : 4 Sep 2020 17:48
Operator : JC/MD
Sample : L3866-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : TOTE-31230

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N083120W.M
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
Benzeneethanamine...	2.42	5.4	ug/l	91599	1	7.63	847412	50.0
Butanal	6.50	7.5	ug/l	127614	1	7.63	847412	50.0
unknown8.25	8.25	8.2	ug/l	214559	2	8.55	1302740	50.0
unknown8.41	8.41	5.3	ug/l	139311	2	8.55	1302740	50.0
3-Buten-2-one, 3-...	8.63	22.6	ug/l	588387	2	8.55	1302740	50.0
2-Pentanone	9.01	6.0	ug/l	157403	2	8.55	1302740	50.0
Pentanal	9.14	11.0	ug/l	286372	2	8.55	1302740	50.0
n-Propyl acetate	9.24	54.3	ug/l	1415140	2	8.55	1302740	50.0
Hexanal	10.83	6.0	ug/l	214850	3	11.38	1781110	50.0