LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN081718\
Data File : VN050733.D
Acq On : 17 Aug 2018 16:27
Operator : MD\SY
Sample : J4545-01
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : RB-BASELINE-WATER

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\82N081418W.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	1.658	3	21	47	rBV	1759353	2934247	82.72%	9.768%
2	1.815	62	70	82	rBV3	29399	46237	1.30%	0.154%
3	2.153	168	175	191	rVB2	36904	59574	1.68%	0.198%
4	3.821	679	694	729	rVB2	225541	602457	16.98%	2.006%
5	4.066	751	770	796	rBV4	26579	90892	2.56%	0.303%
6	4.799	974	998	1022	rBV3	46093	165213	4.66%	0.550%
7	6.561	1527	1546	1562	rBV6	18096	57969	1.63%	0.193%
8	6.844	1611	1634	1657	rBV	87356	256163	7.22%	0.853%
9	7.593	1847	1867	1879	rBV	492881	1248026	35.18%	4.155%
10	7.670	1879	1891	1913	rVB	713069	1671494	47.12%	5.565%
11	8.034	1985	2004	2024	rBV2	561076	1390498	39.20%	4.629%
12	8.233	2046	2066	2067	rBV	37633	93821	2.64%	0.312%
13	8.448	2120	2133	2153	rVB	292051	640163	18.05%	2.131%
14	8.587	2161	2176	2191	rBV	1073014	2211364	62.34%	7.362%
15	8.673	2191	2203	2231	rVB	536621	1139437	32.12%	3.793%
16	9.043	2305	2318	2335	rBV	186189	383809	10.82%	1.278%
17	9.429	2426	2438	2456	rVB2	119508	253835	7.16%	0.845%
18	9.857	2559	2571	2577	rBV	26984	50663	1.43%	0.169%
19	9.895	2577	2583	2595	rVB4	35031	63214	1.78%	0.210%
20	9.988	2600	2612	2622	rBV	93822	182398	5.14%	0.607%
21	10.095	2630	2645	2660	rBV	1926398	3547145	100.00%	11.809%
22	10.197	2669	2677	2692	rVB	102290	198139	5.59%	0.660%
23	10.313	2702	2713	2721	rBV	85317	152760	4.31%	0.509%
24	10.358	2722	2727	2743	rVB5	34355	71365	2.01%	0.238%
25	10.609	2793	2805	2827	rVB	189192	369779	10.42%	1.231%
26	10.757	2831	2851	2873	rBV4	131660	347186	9.79%	1.156%
27	10.905	2887	2897	2907	rBV4	22922	46240	1.30%	0.154%
28	11.069	2935	2948	2959	rBV	98764	174196	4.91%	0.580%
29	11.140	2959	2970	2995	rVB3	114567	221883	6.26%	0.739%
30	11.255	2995	3006	3015	rBV	78615	149362	4.21%	0.497%
31	11.410	3037	3054	3072	rBV	1437187	2538378	71.56%	8.450%
32	11.500	3072	3082	3093	rVV2	165697	361643	10.20%	1.204%
33	11.554	3094	3099	3110	rVV	94136	163798	4.62%	0.545%
34	11.619	3112	3119	3125	rVV4	35135	62662	1.77%	0.209%

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Sample : J4545-01
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : RB-BASELINE-WATER

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

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Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N081418W.M
Title : SW846 8260

35	11.664	3125	3133	3144	rVB	70037	117412	3.31%	0.391%
36	11.779	3159	3169	3176	rBV3	25298	47012	1.33%	0.157%
37	11.850	3183	3191	3203	rVB3	47577	84248	2.38%	0.280%
38	11.947	3213	3221	3232	rVB2	39572	65790	1.85%	0.219%
39	12.033	3239	3248	3256	rBV2	31485	50883	1.43%	0.169%
40	12.104	3259	3270	3277	rVV5	35402	64830	1.83%	0.216%
41	12.156	3278	3286	3306	rVB3	99837	230505	6.50%	0.767%
42	12.275	3312	3323	3331	rBV4	25358	45109	1.27%	0.150%
43	12.361	3341	3350	3353	rBV	82660	120546	3.40%	0.401%
44	12.403	3353	3363	3381	rVB	1235300	2101810	59.25%	6.997%
45	12.574	3409	3416	3423	rBV4	46022	74734	2.11%	0.249%
46	12.657	3435	3442	3448	rBV5	29436	45001	1.27%	0.150%
47	12.728	3456	3464	3475	rVB3	118451	207150	5.84%	0.690%
48	12.808	3477	3489	3498	rBV4	43113	80813	2.28%	0.269%
49	12.889	3509	3514	3524	rVB	31161	48394	1.36%	0.161%
50	12.998	3526	3548	3559	rBV4	111756	342773	9.66%	1.141%
51	13.162	3589	3599	3609	rBV4	47423	86681	2.44%	0.289%
52	13.239	3612	3623	3643	rVV	414634	863069	24.33%	2.873%
53	13.345	3645	3656	3674	rVB	1218863	2224977	62.73%	7.407%
54	13.509	3700	3707	3710	rBV4	26281	36221	1.02%	0.121%
55	13.545	3712	3718	3725	rVB3	51061	68644	1.94%	0.229%
56	13.596	3725	3734	3737	rBV5	66070	101157	2.85%	0.337%
57	13.673	3752	3758	3763	rBV2	35471	46599	1.31%	0.155%
58	13.895	3819	3827	3835	rBV3	32328	49173	1.39%	0.164%
59	13.995	3850	3858	3870	rBV3	62063	106663	3.01%	0.355%
60	14.377	3971	3977	3989	rVB6	38525	59894	1.69%	0.199%
61	14.471	4000	4006	4013	rBV5	34974	49976	1.41%	0.166%
62	14.522	4015	4022	4032	rVV6	58234	98593	2.78%	0.328%
63	14.583	4033	4041	4053	rVB5	62559	141664	3.99%	0.472%
64	14.657	4056	4064	4072	rBV8	51183	93316	2.63%	0.311%
65	14.744	4084	4091	4105	rVB3	66243	117405	3.31%	0.391%
66	15.133	4206	4212	4224	rVB	98437	168527	4.75%	0.561%
67	16.355	4585	4592	4602	rVB2	28379	52949	1.49%	0.176%

Sum of corrected areas: 30038528

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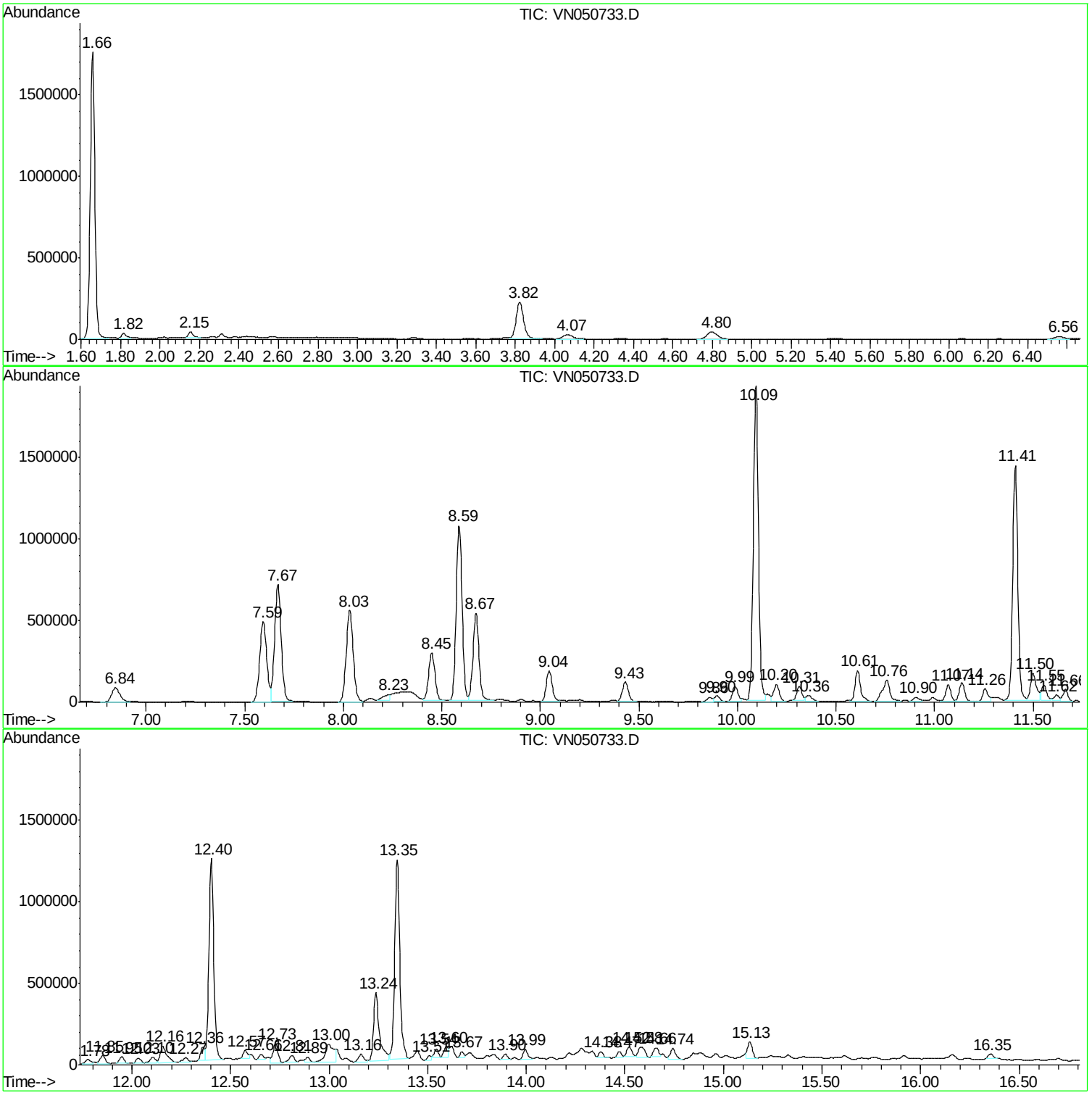
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
RB-BASELINE-WATER

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N081418W.M
Quant Title : SW846 8260

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



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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N081418W.M
Quant Title : SW846 8260

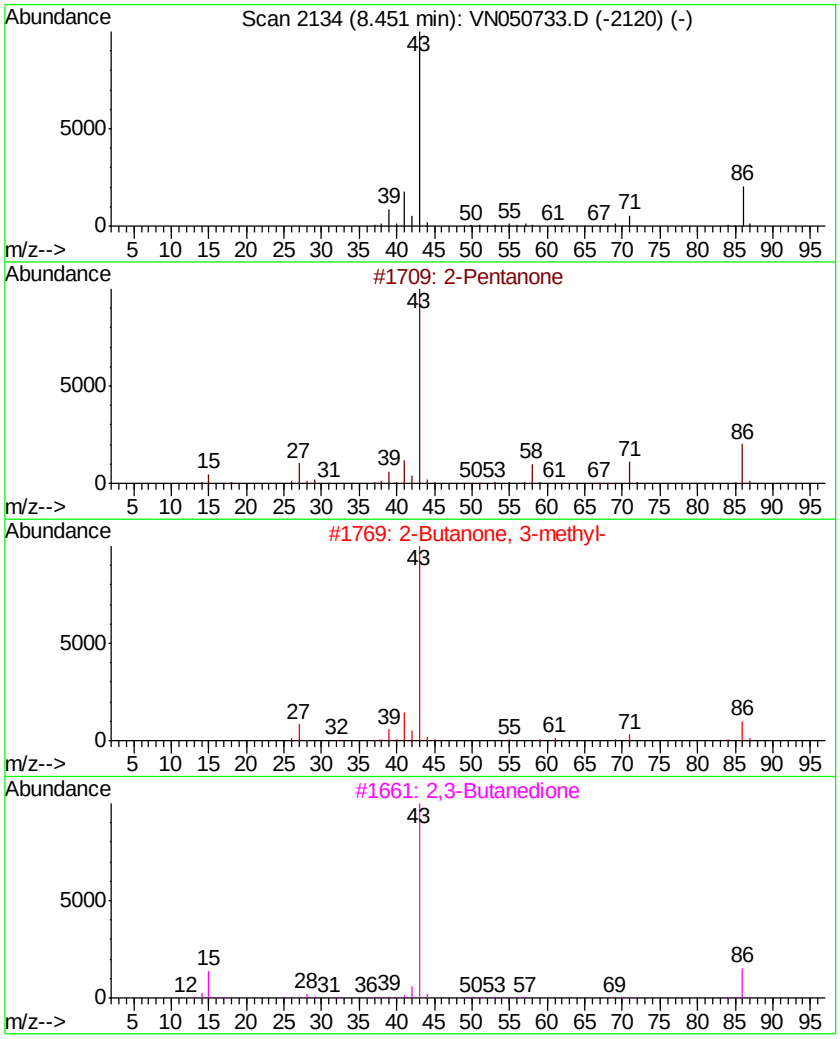
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

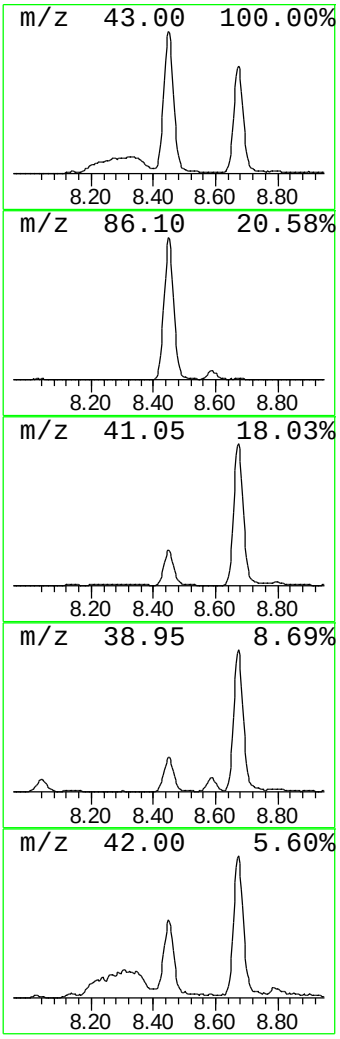
****

Peak Number 2 2-Pentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.45	14.47 ug/l	640163	1,4-Difluorobenzene	8.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	64
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	64
3	2,3-Butanedione	86	C4H6O2	000431-03-8	59
4	2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	9
5	2,3-Hexanedione	114	C6H10O2	003848-24-6	9





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN081718\
Data File : VN050733.D
Acq On : 17 Aug 2018 16:27
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Sample : J4545-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : RB-BASELINE-WATER

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N081418W.M
Quant Title : SW846 8260

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

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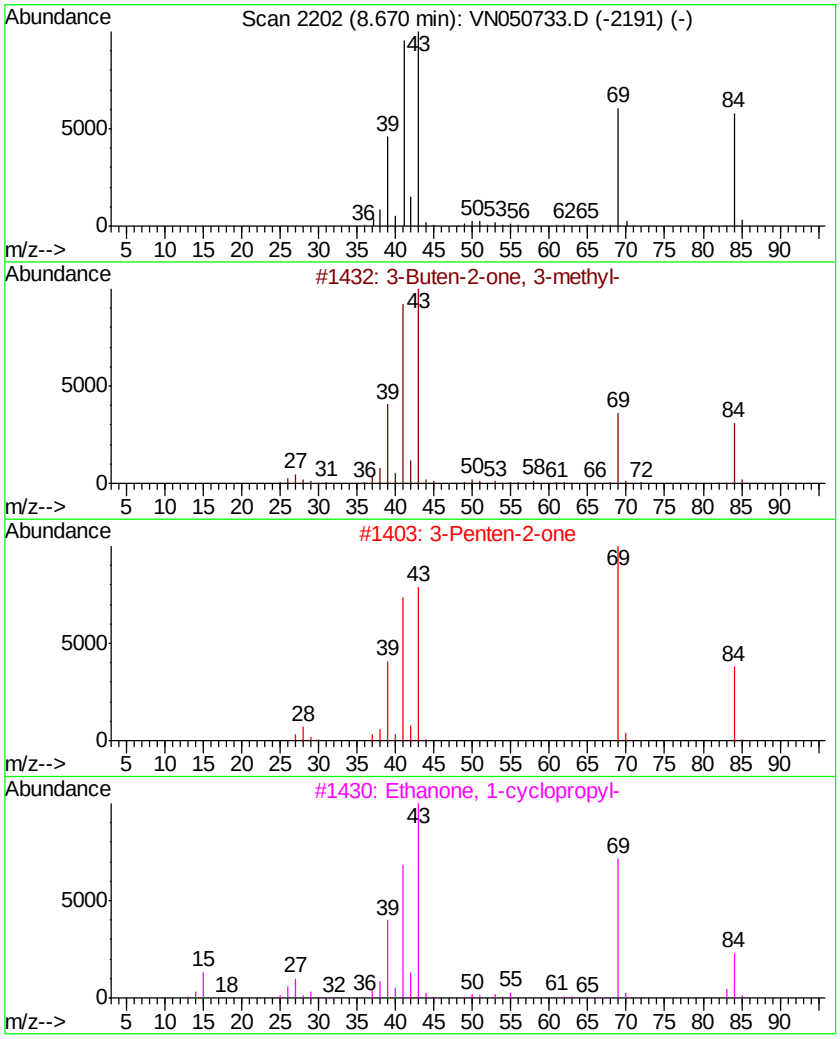
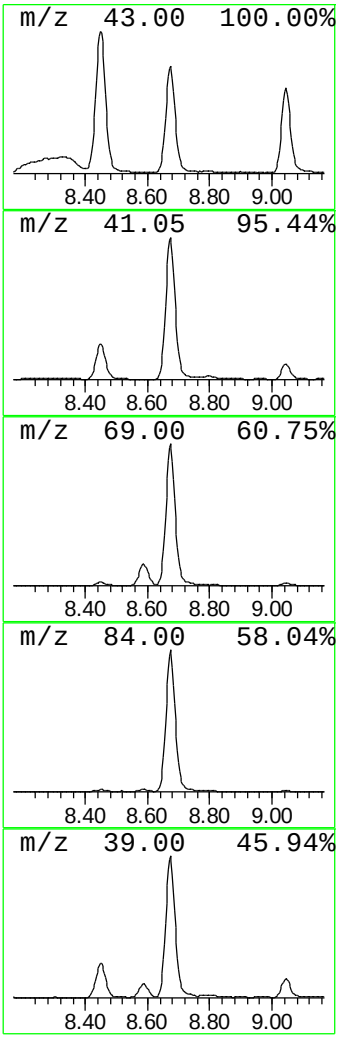
Peak Number 3 3-Buten-2-one, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.67	25.76 ug/l	1139440	1,4-Difluorobenzene	8.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-2-one, 3-methyl-	84	C5H8O	000814-78-8	91
2	3-Penten-2-one	84	C5H8O	000625-33-2	90
3	Ethanone, 1-cyclopropyl-	84	C5H8O	000765-43-5	64
4	2-Butanone, 4-hydroxy-3-(hydroxy...	132	C6H12O3	006868-97-9	36
5	3-Penten-2-one, (E)-	84	C5H8O	003102-33-8	35





Library Search Compound Report

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Data File : VN050733.D
Acq On : 17 Aug 2018 16:27
Operator : MD\SY
Sample : J4545-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : RB-BASELINE-WATER

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N081418W.M
Quant Title : SW846 8260

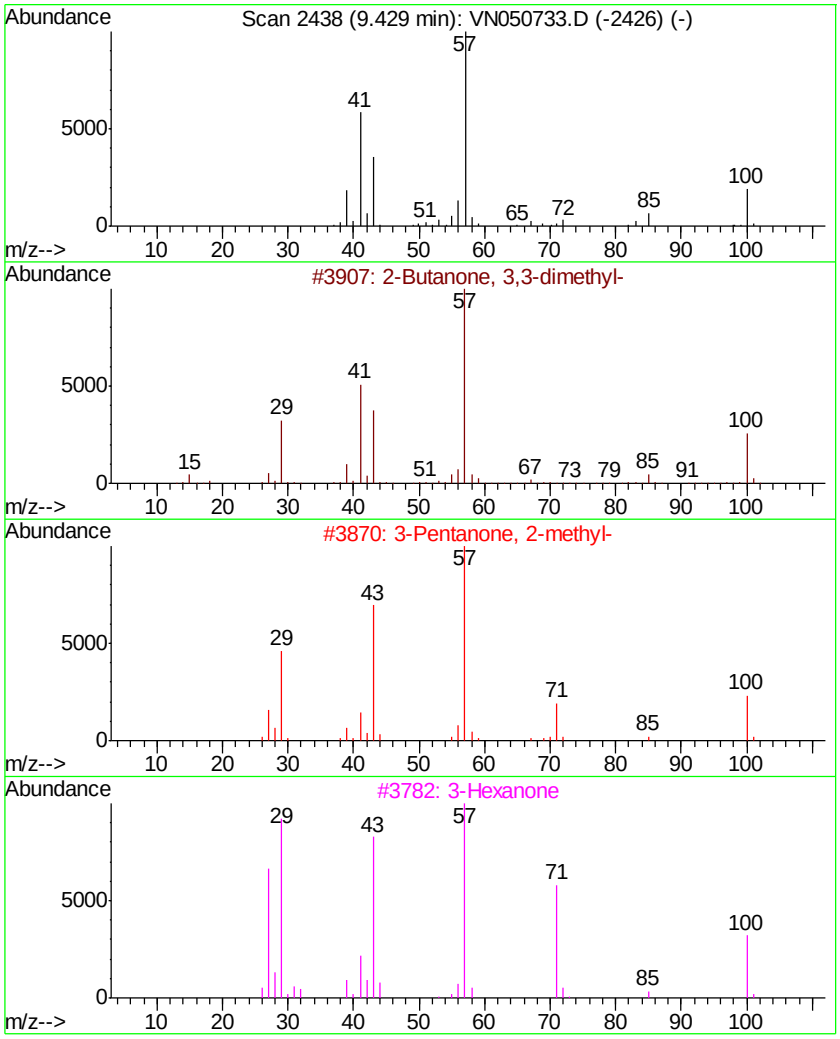
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

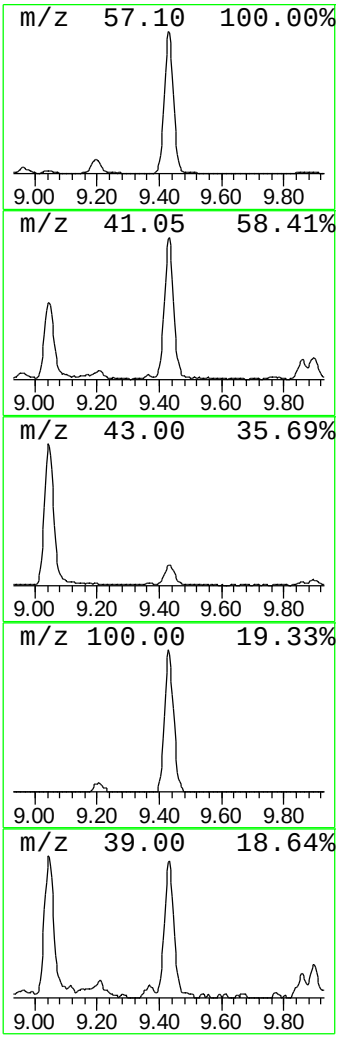
****

Peak Number 5 2-Butanone, 3,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.43	5.74 ug/l	253835	1,4-Difluorobenzene	8.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	72
2	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	50
3	3-Hexanone	100	C6H12O	000589-38-8	37
4	Butane, 2-bromo-	136	C4H9Br	000078-76-2	37
5	Oxalic acid, butyl propyl ester	188	C9H16O4	1000309-25-6	37





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN081718\
Data File : VN050733.D
Acq On : 17 Aug 2018 16:27
Operator : MD\SY
Sample : J4545-01
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : RB-BASELINE-WATER

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N081418W.M
Quant Title : SW846 8260

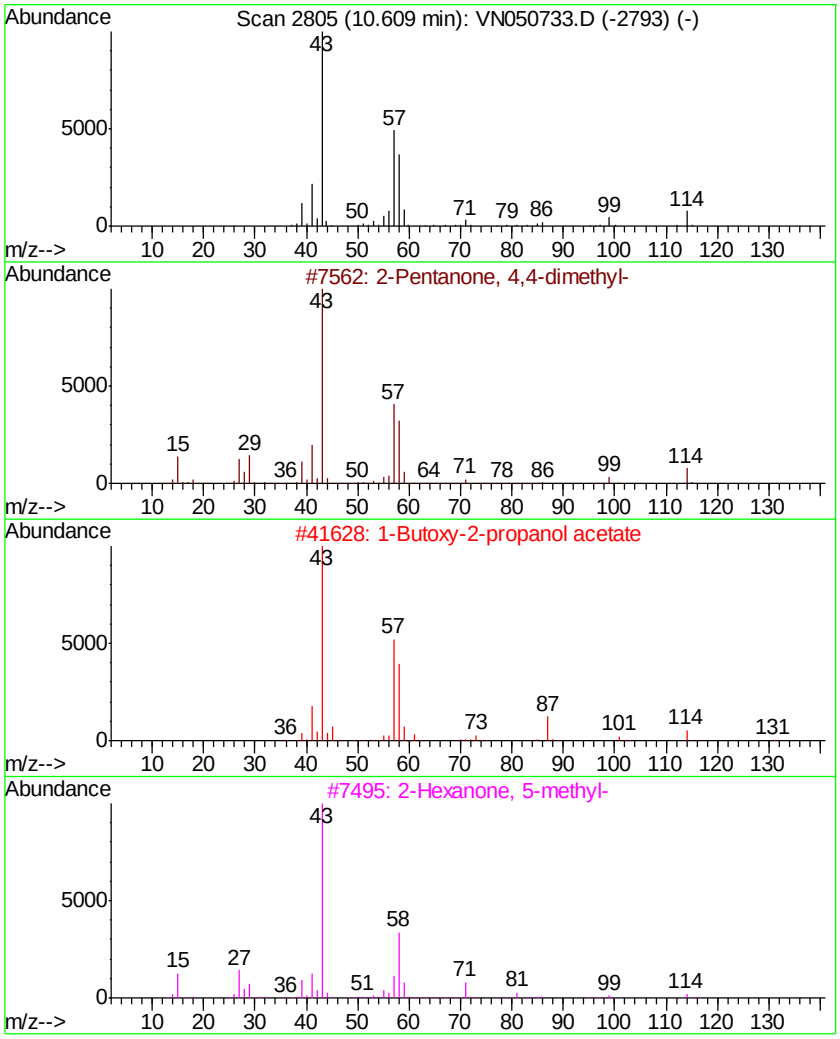
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

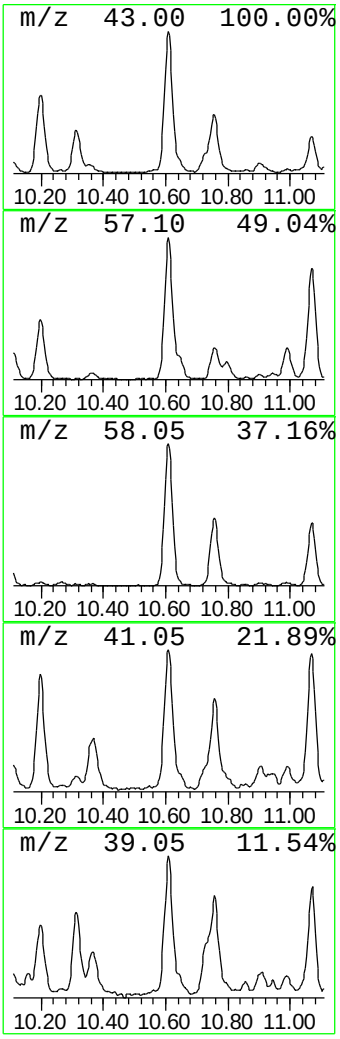
****

Peak Number 6 2-Pentanone, 4,4-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.61	7.28 ug/l	369779	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	90
2	1-Butoxy-2-propanol acetate	174	C9H18O3	085409-76-3	64
3	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	56
4	3-Oxetanol, 2,2,3-trimethyl-	116	C6H12O2	025910-96-7	38
5	2-Nonanone	142	C9H18O	000821-55-6	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN081718\
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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
2-Pentanone	8.45	14.5	ug/l	640163	2	8.59	2211360	50.0
3-Buten-2-one, 3-...	8.67	25.8	ug/l	1139440	2	8.59	2211360	50.0
2-Butanone, 3,3-d...	9.43	5.7	ug/l	253835	2	8.59	2211360	50.0
2-Pentanone, 4,4-...	10.61	7.3	ug/l	369779	3	11.41	2538380	50.0