LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN082520\
Data File : VN063118.D
Acq On : 25 Aug 2020 17:51
Operator : JC/MD
Sample : L3788-03
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 1794

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\82N081820W.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	3.780	602	624	674	rBV	2132947	6000039	100.00%	27.999%
2	4.024	685	700	727	rVB	116735	342937	5.72%	1.600%
3	4.294	770	784	808	rVB2	32597	99270	1.65%	0.463%
4	4.735	892	921	962	rBV	405332	1435518	23.93%	6.699%
5	6.503	1450	1471	1493	rBV4	36383	122712	2.05%	0.573%
6	6.786	1537	1559	1594	rBV	653166	1911107	31.85%	8.918%
7	7.153	1656	1673	1695	rBV3	26869	77330	1.29%	0.361%
8	7.551	1778	1797	1808	rBV2	102971	257674	4.29%	1.202%
9	7.628	1808	1821	1844	rVB2	188558	450505	7.51%	2.102%
10	7.989	1910	1933	1953	rBV2	135235	344016	5.73%	1.605%
11	8.252	1987	2015	2051	rBV5	66619	426537	7.11%	1.990%
12	8.410	2053	2064	2083	rVB2	125837	294761	4.91%	1.376%
13	8.551	2095	2108	2126	rVB	303597	624282	10.40%	2.913%
14	9.008	2236	2250	2266	rBV	408205	800713	13.35%	3.737%
15	9.156	2279	2296	2318	rVB3	72852	209067	3.48%	0.976%
16	9.397	2356	2371	2398	rVB	1102622	2243822	37.40%	10.471%
17	9.956	2531	2545	2556	rBV	58392	110031	1.83%	0.513%
18	10.062	2560	2578	2596	rVB	496853	1033156	17.22%	4.821%
19	10.165	2601	2610	2623	rVB	40995	79723	1.33%	0.372%
20	10.378	2655	2676	2689	rVB9	46869	120689	2.01%	0.563%
21	10.580	2728	2739	2744	rBV	37541	68683	1.14%	0.321%
22	10.612	2745	2749	2768	rVB	47141	73725	1.23%	0.344%
23	10.725	2768	2784	2806	rBV	182224	366900	6.11%	1.712%
24	10.828	2806	2816	2828	rVB	118143	195548	3.26%	0.913%
25	10.927	2839	2847	2862	rVB	45616	88073	1.47%	0.411%
26	11.381	2976	2988	3000	rBV	453929	805419	13.42%	3.759%
27	11.554	3033	3042	3051	rVV5	34049	62643	1.04%	0.292%
28	11.635	3062	3067	3076	rVB	50464	76560	1.28%	0.357%
29	11.696	3077	3086	3098	rBV4	63688	121978	2.03%	0.569%
30	11.789	3107	3115	3122	rBV	44609	73199	1.22%	0.342%
31	12.005	3170	3182	3199	rBV	167000	278380	4.64%	1.299%
32	12.104	3203	3213	3233	rBV7	57120	122747	2.05%	0.573%
33	12.313	3270	3278	3287	rVB	40205	64857	1.08%	0.303%
34	12.378	3287	3298	3310	rBV	362054	603431	10.06%	2.816%

LSC Area Percent Report

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Title : SW846 8260

35	12.705	3391	3400	3409	rBV	96954	144829	2.41%	0.676%
36	12.860	3442	3448	3465	rVB5	41341	68916	1.15%	0.322%
37	12.950	3467	3476	3491	rBV5	40078	91078	1.52%	0.425%
38	13.066	3504	3512	3520	rVB2	51726	76918	1.28%	0.359%
39	13.168	3537	3544	3566	rVB4	32440	61553	1.03%	0.287%
40	13.320	3578	3591	3604	rBV	433580	719739	12.00%	3.359%
41	13.426	3615	3624	3636	rVB5	32920	66545	1.11%	0.311%
42	13.799	3732	3740	3755	rVB3	41379	77300	1.29%	0.361%
43	14.648	3995	4004	4019	rVB2	44973	74264	1.24%	0.347%
44	15.474	4252	4261	4275	rVB2	36300	62001	1.03%	0.289%

Sum of corrected areas: 21429175

LSC Report - Integrated Chromatogram

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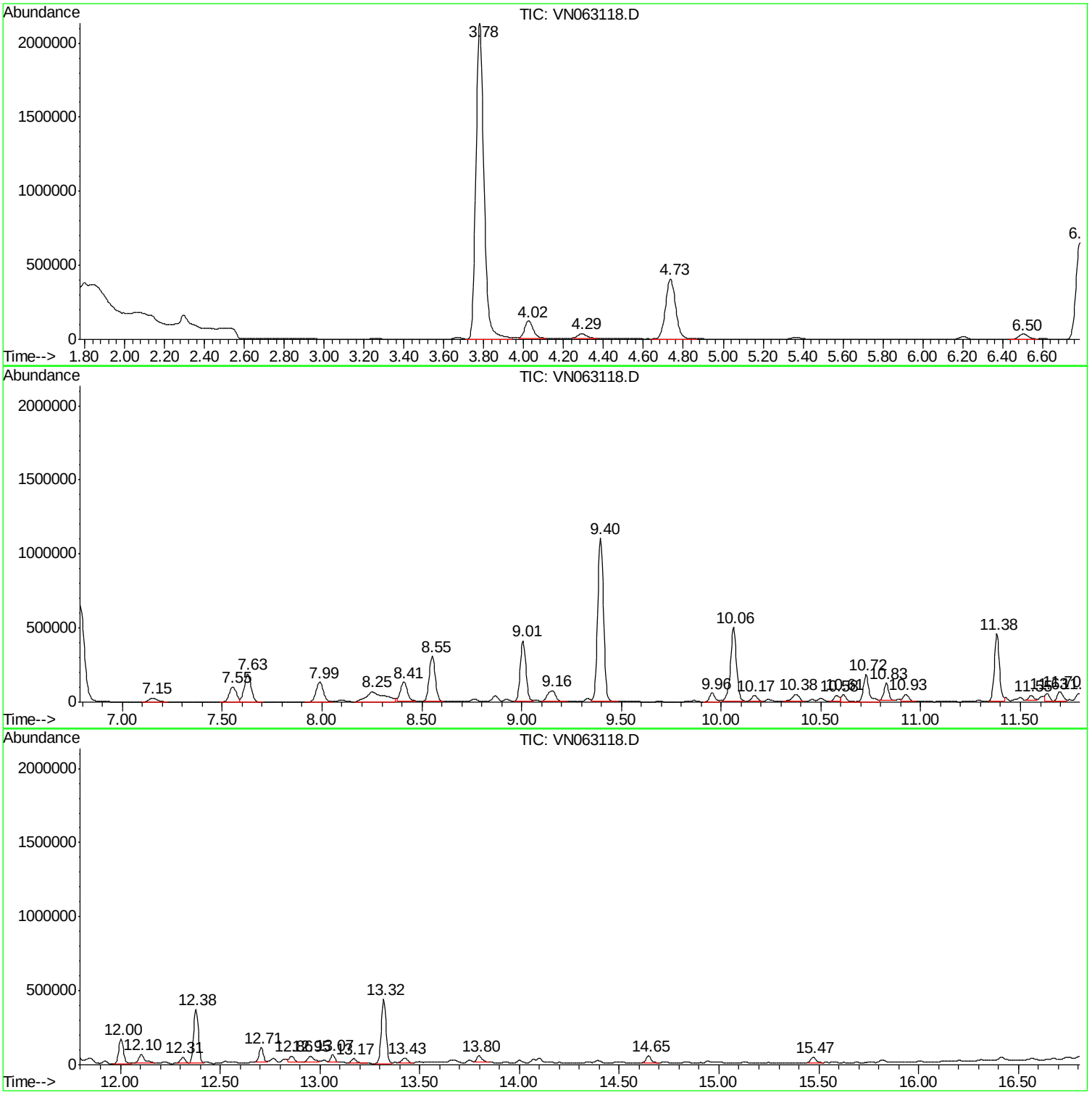
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N081820W.M
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

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Peak Number 1 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.02	38.06 ug/l	342937	Pentafluorobenzene	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	86
2	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	43
3	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
4	(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	9
5	2-Pentanol	88	C5H12O	006032-29-7	9

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Peak Number 2 Butanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	13.62 ug/l	122712	Pentafluorobenzene	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	58
2	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	47
3	Allyl ethyl ether	86	C5H10O	000557-31-3	35
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	32
5	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	28

****

Peak Number 3 Acetic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.25	34.16 ug/l	426537	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	52
2	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	38
3	Ethylamine	45	C2H7N	000075-04-7	37
4	Formic acid, 2-methylpropyl ester	102	C5H10O2	000542-55-2	12
5	5-Hexen-2-ol	100	C6H12O	000626-94-8	10

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Peak Number 4 2-Butanone, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.

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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 1794

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N081820W.M
Quant Title : SW846 8260

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.41	23.61 ug/l	294761	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	59
2	2,3-Butanedione	86	C4H6O2	000431-03-8	58
3	2-Pentanone	86	C5H10O	000107-87-9	53
4	Isobutane	58	C4H10	000075-28-5	9
5	3,3-Dimethyl-2,4-pentane dione	128	C7H12O2	003142-58-3	9

****

Peak Number 5 2-Pentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.01	64.13 ug/l	800713	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	91
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	53
3	2,3-Butanedione	86	C4H6O2	000431-03-8	9
4	Butane	58	C4H10	000106-97-8	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9

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Peak Number 6 3-Pentanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.16	16.74 ug/l	209067	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	72
2	Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	9
3	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	9
4	Isobutyl ether	130	C8H18O	000628-55-7	9
5	Neopentane	72	C5H12	000463-82-1	9

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Peak Number 7 2-Butanone, 3,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.40	179.71 ug/l	2243820	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual

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Instrument : MSVOA_N
ClientSampleId : 1794

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N081820W.M
Quant Title : SW846 8260

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

1	2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	86
2	3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	58
3	3-Hexanone	100	C6H12O	000589-38-8	42
4	Neopentane	72	C5H12	000463-82-1	38
5	Propanoic acid, 2,2-dimethyl-, s...	208	C5H9AgO2	007324-58-5	38

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Peak Number 8 Hexanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.83	12.14 ug/l	195548	Chlorobenzene-d5	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	93
2	Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	38
3	Cyclopentanol, 2-methyl-, cis-	100	C6H12O	025144-05-2	35
4	Butanal	72	C4H8O	000123-72-8	35
5	2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	32

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Peak Number 9 2-Heptanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.00	17.28 ug/l	278380	Chlorobenzene-d5	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone	114	C7H14O	000110-43-0	91
2	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	90
3	2-Octanone	128	C8H16O	000111-13-7	72
4	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	64
5	2-Pentanone, 4,4-dimethyl-	114	C7H14O	000590-50-1	52

****

Peak Number 10 2-Heptanone, 6-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	10.06 ug/l	144829	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone, 6-methyl-	128	C8H16O	000928-68-7	91
2	2-Isopropyl-5-oxohexanal	156	C9H16O2	015303-46-5	56
3	2-Heptanone, 4-methyl-	128	C8H16O	006137-06-0	53

Library Search Compound Report

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

4	2-Heptanone	114	C7H14O	000110-43-0	53
5	Pentanal, 2-methyl-	100	C6H12O	000123-15-9	50

Tentatively Identified Compound (LSC) summary

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Quant Title : SW846 8260

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Isopropyl Alcohol	4.02	38.1	ug/l	342937	1	7.63	450505	50.0
Butanal	6.50	13.6	ug/l	122712	1	7.63	450505	50.0
Acetic acid	8.25	34.2	ug/l	426537	2	8.55	624282	50.0
2-Butanone, 3-met...	8.41	23.6	ug/l	294761	2	8.55	624282	50.0
2-Pentanone	9.01	64.1	ug/l	800713	2	8.55	624282	50.0
3-Pentanone	9.16	16.7	ug/l	209067	2	8.55	624282	50.0
2-Butanone, 3,3-d...	9.40	179.7	ug/l	2243820	2	8.55	624282	50.0
Hexanal	10.83	12.1	ug/l	195548	3	11.38	805419	50.0
2-Heptanone	12.00	17.3	ug/l	278380	3	11.38	805419	50.0
2-Heptanone, 6-me...	12.71	10.1	ug/l	144829	4	13.32	719739	50.0