LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN082520\
Data File : VN063120.D
Acq On : 25 Aug 2020 18:39
Operator : JC/MD
Sample : L3792-06
Misc : 5.00mL/MSVOA N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP-1

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	3.249	442	459	504	rBV	80986	271008	29.78%	2.706%
2	3.783	603	625	660	rBV	191160	536338	58.94%	5.356%
3	4.027	684	701	724	rBV	65392	196593	21.60%	1.963%
4	4.291	770	783	810	rVB	32877	99028	10.88%	0.989%
5	4.738	898	922	956	rVB	53997	212284	23.33%	2.120%
6	5.905	1266	1285	1287	rBV5	8205	16769	1.84%	0.167%
7	6.493	1449	1468	1469	rBV4	6316	13861	1.52%	0.138%
8	6.783	1539	1558	1581	rBV3	25493	82637	9.08%	0.825%
9	7.551	1780	1797	1808	rBV2	104575	255700	28.10%	2.553%
10	7.628	1808	1821	1845	rVB	191813	456828	50.20%	4.562%
11	7.998	1912	1936	1953	rBV3	209824	555653	61.06%	5.549%
12	8.091	1957	1965	1988	rVB5	11277	29421	3.23%	0.294%
13	8.271	1991	2021	2022	rBV3	34813	124484	13.68%	1.243%
14	8.554	2093	2109	2127	rVB	304286	635880	69.88%	6.350%
15	8.760	2163	2173	2189	rBV4	5628	12322	1.35%	0.123%
16	9.008	2239	2250	2263	rBV3	9374	19716	2.17%	0.197%
17	9.168	2290	2300	2314	rVB5	7846	19241	2.11%	0.192%
18	9.548	2405	2418	2429	rBV3	5436	11720	1.29%	0.117%
19	9.680	2449	2459	2471	rBV	14320	25265	2.78%	0.252%
20	9.956	2535	2545	2562	rVB	30047	54358	5.97%	0.543%
21	10.062	2563	2578	2589	rBV	490877	895833	98.44%	8.946%
22	10.127	2589	2598	2620	rVB	152763	286443	31.48%	2.860%
23	10.329	2653	2661	2673	rVB3	20279	35781	3.93%	0.357%
24	10.779	2793	2801	2809	rBV	13929	23421	2.57%	0.234%
25	10.850	2809	2823	2835	rVB9	15450	45077	4.95%	0.450%
26	11.381	2975	2988	3010	rVB	458806	806868	88.67%	8.057%
27	11.509	3010	3028	3035	rBV5	25395	66000	7.25%	0.659%
28	11.557	3036	3043	3047	rVV3	31271	50218	5.52%	0.501%
29	11.593	3047	3054	3076	rVB	93678	174329	19.16%	1.741%
30	11.699	3076	3087	3093	rBV	18234	33272	3.66%	0.332%
31	11.828	3116	3127	3140	rBV2	11365	25533	2.81%	0.255%
32	11.927	3147	3158	3169	rBV5	55891	115828	12.73%	1.157%
33	12.175	3224	3235	3241	rBV3	10790	19180	2.11%	0.192%
34	12.377	3286	3298	3309	rBV	387834	646361	71.03%	6.455%

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Title : SW846 8260

35	12.435	3310	3316	3328	rVB2	30129	49565	5.45%	0.495%
36	12.570	3350	3358	3370	rVB2	13929	22345	2.46%	0.223%
37	12.638	3370	3379	3382	rBV2	7402	11380	1.25%	0.114%
38	12.885	3450	3456	3467	rVB7	16365	29051	3.19%	0.290%
39	13.017	3487	3497	3506	rBV	65611	101466	11.15%	1.013%
40	13.075	3508	3515	3524	rVB6	17758	30812	3.39%	0.308%
41	13.319	3579	3591	3608	rBV	479264	812219	89.26%	8.111%
42	13.426	3616	3624	3642	rVB2	56199	103097	11.33%	1.030%
43	13.522	3647	3654	3672	rVB6	15589	32565	3.58%	0.325%
44	13.699	3698	3709	3722	rBV	265034	438526	48.19%	4.379%
45	13.821	3732	3747	3770	rVB	20226	69331	7.62%	0.692%
46	13.943	3777	3785	3789	rBV8	8981	14636	1.61%	0.146%
47	14.069	3814	3824	3831	rBV2	28921	57855	6.36%	0.578%
48	14.194	3857	3863	3873	rVB5	14084	18656	2.05%	0.186%
49	14.641	3993	4002	4014	rVB6	45259	84975	9.34%	0.849%
50	14.715	4020	4025	4042	rVB3	25369	43861	4.82%	0.438%
51	14.821	4052	4058	4067	rVB5	24151	36962	4.06%	0.369%
52	15.107	4134	4147	4161	rBV	508229	909985	100.00%	9.087%
53	15.470	4253	4260	4270	rBV3	28400	48636	5.34%	0.486%
54	16.126	4455	4464	4477	rVB	52728	103565	11.38%	1.034%
55	16.210	4481	4490	4509	rVB5	29195	70397	7.74%	0.703%
56	16.316	4514	4523	4536	rVB2	36857	70763	7.78%	0.707%

Sum of corrected areas: 10013898

LSC Report - Integrated Chromatogram

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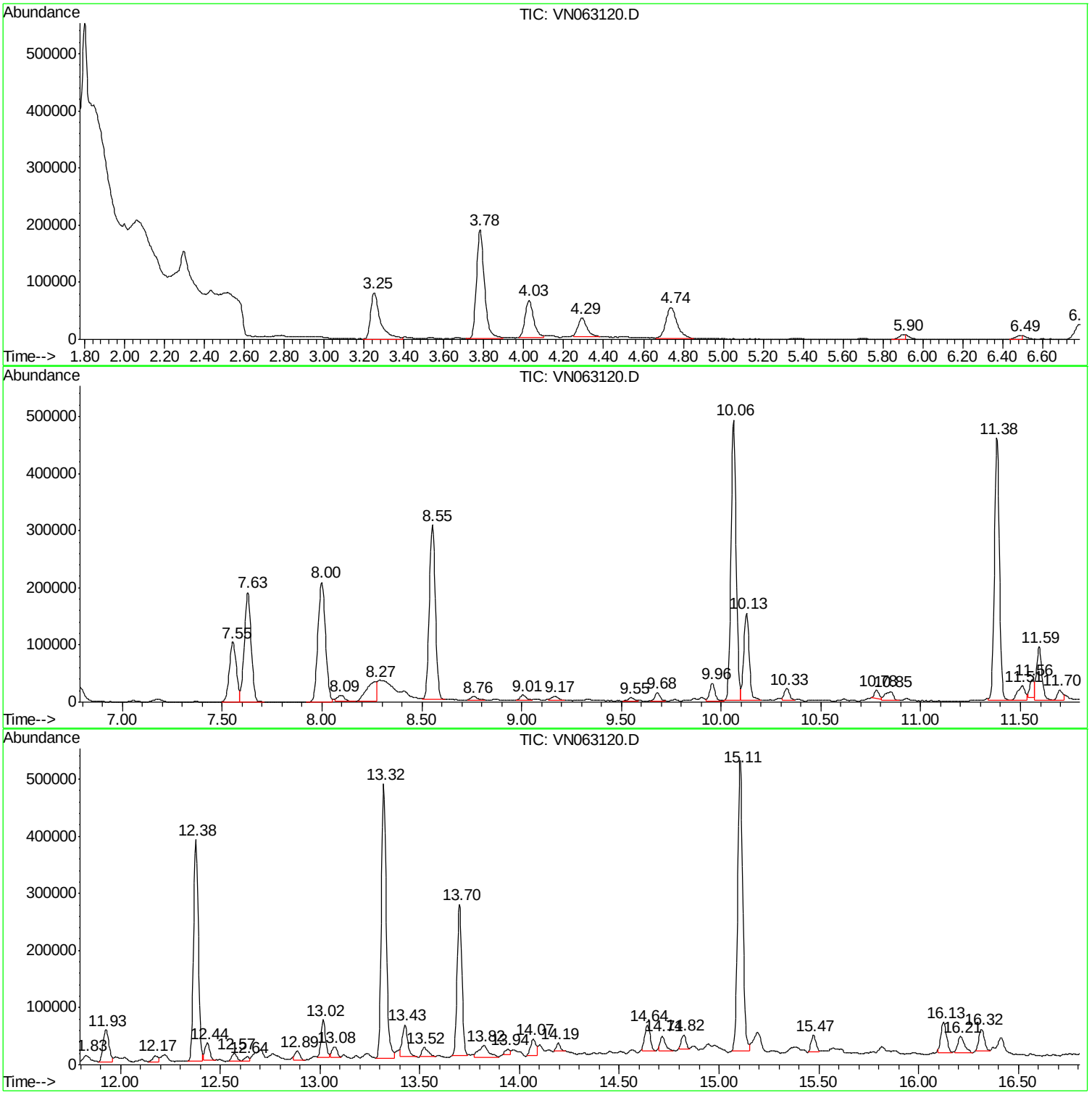
Instrument : MSVOA_N
ClientSampleId : COMP-1

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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TIC Integration Parameters: LSCINT.P

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Peak Number 1 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.25	29.66 ug/l	271008	Pentafluorobenzene	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	64
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Formic acid	46	CH2O2	000064-18-6	4
4	Oxalic acid	90	C2H2O4	000144-62-7	4
5	1-Pyrroline, 2-phenyl-	145	C10H11N	000700-91-4	4

****

Peak Number 2 Acetic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.27	9.79 ug/l	124484	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	90
2	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	50
3	Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	9
4	Formic acid hydrazide	60	CH4N2O	000624-84-0	9
5	Ammonium acetate	77	C2H7NO2	000631-61-8	9

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Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	6.35 ug/l	103097	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
3	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
4	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7	47
5	Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	47

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Peak Number 4 Indene Concentration Rank 2

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

Library Search Compound Report

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Instrument : MSVOA_N
ClientSampleId : COMP-1

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.
13.70	27.00 ug/l	438526	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	97
2	Benzene, 1-propynyl-	116	C9H8	000673-32-5	94
3	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91
5	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	90

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Peak Number 5 2a,4a,6a,6b-Tetrahydrocyclo... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	5.23 ug/l	84975	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2a,4a,6a,6b-Tetrahydrocyclopenta...	130	C10H10	006053-74-3	70
2	Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	64
3	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	64
4	1,4-Dihydronaphthalene	130	C10H10	000612-17-9	55
5	Naphthalene, 1,2-dihydro-	130	C10H10	000447-53-0	55

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Peak Number 6 Naphthalene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.13	6.38 ug/l	103565	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
4	Benzocycloheptatriene	142	C11H10	000264-09-5	90
5	Spiro(tricyclo[6.2.1.0(2,7)]unde...	186	C13H14O	1000210-02-3	78

Tentatively Identified Compound (LSC) summary

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Instrument : MSVOA_N
ClientSampleId : COMP-1

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol	3.25	29.7	ug/l	271008	1	7.63	456828	50.0
Acetic acid	8.27	9.8	ug/l	124484	2	8.55	635880	50.0
1-Hexanol, 2-ethyl-	13.43	6.3	ug/l	103097	4	13.32	812219	50.0
Indene	13.70	27.0	ug/l	438526	4	13.32	812219	50.0
2a,4a,6a,6b-Tetra...	14.64	5.2	ug/l	84975	4	13.32	812219	50.0
Naphthalene, 1-me...	16.13	6.4	ug/l	103565	4	13.32	812219	50.0