LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN082520\
Data File : VN063122.D
Acq On : 25 Aug 2020 19:28
Operator : JC/MD
Sample : L3792-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : COMP-3

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	1.799	3	8	20	rVB	308499	374420	24.98%	3.028%
2	3.253	443	460	478	rBV2	8185	25266	1.69%	0.204%
3	3.780	607	624	660	rBV	226911	626753	41.82%	5.069%
4	4.024	683	700	725	rBV	72555	214586	14.32%	1.736%
5	4.288	768	782	810	rVB	32589	100457	6.70%	0.813%
6	4.735	899	921	957	rVB2	62223	244403	16.31%	1.977%
7	5.905	1268	1285	1305	rVB5	8417	27405	1.83%	0.222%
8	6.490	1451	1467	1487	rBV8	6927	23782	1.59%	0.192%
9	6.783	1536	1558	1581	rBV3	25243	86304	5.76%	0.698%
10	7.172	1662	1679	1695	rVB8	5484	17866	1.19%	0.145%
11	7.333	1715	1729	1749	rBV3	6780	19229	1.28%	0.156%
12	7.551	1779	1797	1808	rBV2	109891	274636	18.33%	2.221%
13	7.629	1808	1821	1844	rVB	206909	492210	32.84%	3.981%
14	7.998	1917	1936	1955	rBV4	283264	748197	49.92%	6.052%
15	8.265	1986	2019	2020	rBV3	22832	70640	4.71%	0.571%
16	8.551	2094	2108	2126	rVB	323593	671354	44.80%	5.430%
17	9.008	2239	2250	2261	rBV4	9950	21395	1.43%	0.173%
18	9.169	2289	2300	2315	rVB3	8510	21644	1.44%	0.175%
19	9.680	2448	2459	2471	rBV2	13781	25346	1.69%	0.205%
20	9.953	2534	2544	2563	rVB	42550	80107	5.35%	0.648%
21	10.063	2563	2578	2589	rBV	533140	959896	64.05%	7.764%
22	10.127	2589	2598	2624	rVB	241638	442651	29.54%	3.580%
23	10.326	2652	2660	2673	rVB	25321	42226	2.82%	0.342%
24	10.776	2791	2800	2808	rBV	15437	26186	1.75%	0.212%
25	10.850	2808	2823	2834	rVB6	17251	51984	3.47%	0.420%
26	11.381	2976	2988	3004	rVB	487242	827451	55.21%	6.693%
27	11.506	3009	3027	3035	rBV4	24636	72290	4.82%	0.585%
28	11.558	3035	3043	3046	rVV3	35200	51084	3.41%	0.413%
29	11.593	3046	3054	3075	rVB	117815	230285	15.37%	1.863%
30	11.696	3076	3086	3094	rBV2	21367	39997	2.67%	0.324%
31	11.927	3147	3158	3170	rBV4	75185	154457	10.31%	1.249%
32	12.175	3226	3235	3241	rBV5	12653	21739	1.45%	0.176%
33	12.378	3284	3298	3309	rBV	399132	671537	44.81%	5.431%
34	12.435	3309	3316	3327	rVB	38414	62707	4.18%	0.507%

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Title : SW846 8260

35	12.570	3349	3358	3369	rBV2	15205	25769	1.72%	0.208%
36	12.635	3371	3378	3383	rBV	9506	15238	1.02%	0.123%
37	12.886	3446	3456	3469	rVB9	15658	35840	2.39%	0.290%
38	13.017	3488	3497	3507	rVV	76882	133059	8.88%	1.076%
39	13.075	3508	3515	3524	rVV6	24628	47492	3.17%	0.384%
40	13.236	3557	3565	3578	rVB4	12760	24048	1.60%	0.195%
41	13.320	3578	3591	3607	rBV	481102	842160	56.19%	6.811%
42	13.426	3610	3624	3640	rVB4	45716	129358	8.63%	1.046%
43	13.522	3646	3654	3675	rBV4	21197	52911	3.53%	0.428%
44	13.699	3692	3709	3724	rBV	392267	661507	44.14%	5.350%
45	13.821	3732	3747	3768	rVB10	25082	83145	5.55%	0.672%
46	13.937	3774	3783	3803	rBV7	15408	45805	3.06%	0.370%
47	14.069	3814	3824	3831	rBV2	34243	66879	4.46%	0.541%
48	14.194	3856	3863	3875	rVB3	17090	28023	1.87%	0.227%
49	14.638	3990	4001	4014	rBV3	44395	93325	6.23%	0.755%
50	14.715	4018	4025	4037	rVB2	29298	47861	3.19%	0.387%
51	14.824	4049	4059	4066	rBV6	33440	57880	3.86%	0.468%
52	14.866	4067	4072	4084	rVB5	23933	38042	2.54%	0.308%
53	15.104	4133	4146	4161	rBV	847699	1498644	100.00%	12.121%
54	15.197	4165	4175	4189	rVB	44685	98049	6.54%	0.793%
55	15.471	4252	4260	4272	rBV3	25729	43698	2.92%	0.353%
56	15.818	4361	4368	4375	rVB8	10011	15733	1.05%	0.127%
57	16.123	4452	4463	4476	rBV	94713	187840	12.53%	1.519%
58	16.210	4480	4490	4510	rVB3	39327	97785	6.52%	0.791%
59	16.316	4511	4523	4535	rBV	59958	124443	8.30%	1.007%
60	16.413	4546	4553	4566	rVB3	24544	48800	3.26%	0.395%

Sum of corrected areas: 12363824

LSC Report - Integrated Chromatogram

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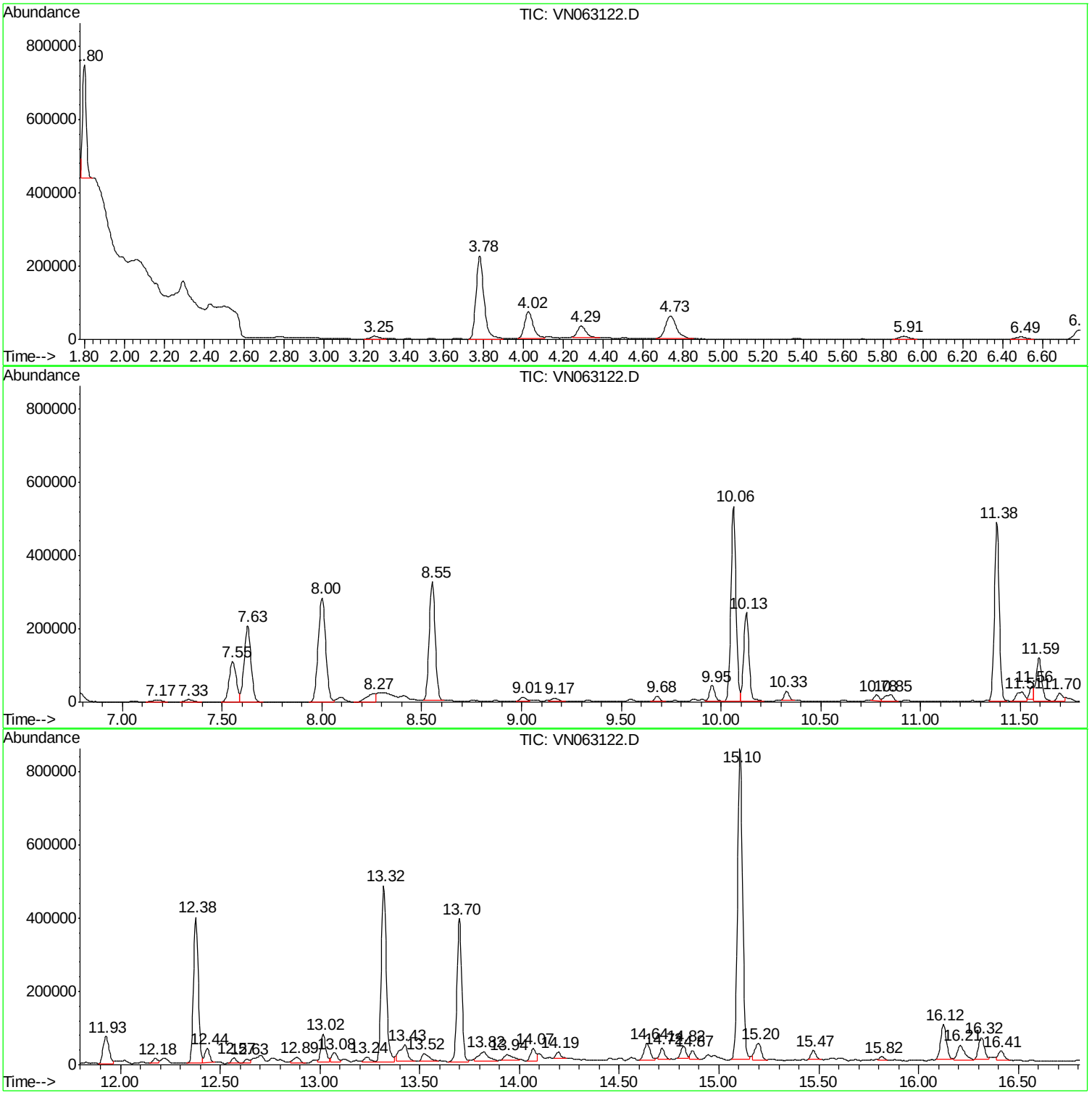
ClientSampleId : COMP-3

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

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

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Peak Number 1 Propane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.80	38.03 ug/l	374420	Pentafluorobenzene	7.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	74
2	Propene	42	C3H6	000115-07-1	9
3	Cyclopropene	40	C3H4	002781-85-3	2
4	Cyclobutylamine	71	C4H9N	002516-34-9	2
5	Pyrimidine-2,4(1H,3H)-dione, 5-a...	156	C4H4N4O3	1000270-67-7	2

****

Peak Number 2 Acetic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.27	5.26 ug/l	70640	1,4-Difluorobenzene	8.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid	60	C2H4O2	000064-19-7	83
2	Formic acid hydrazide	60	CH4N2O	000624-84-0	9
3	Ammonium acetate	77	C2H7NO2	000631-61-8	9
4	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	7
5	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	5

****

Peak Number 3 unknown13.43 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.43	7.68 ug/l	129358	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	47
2	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	42
3	Oxalic acid, butyl 2-ethylhexyl ...	258	C14H26O4	1000309-38-6	40
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	40
5	Oxalic acid, 2-ethylhexyl isobut...	258	C14H26O4	1000309-38-5	40

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Peak Number 4 Indene Concentration Rank 1

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

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Instrument : MSVOA_N
ClientSampleId : COMP-3

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

13.70	39.27 ug/l	661507	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	91
3	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
4	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
5	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	91

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Peak Number 5 2-Methylindene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	5.54 ug/l	93325	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylindene	130	C10H10	002177-47-1	96
2	1H-Indene, 1-methyl-	130	C10H10	000767-59-9	94
3	Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	93
4	1,4-Dihydronaphthalene	130	C10H10	000612-17-9	92
5	1H-Indene, 3-methyl-	130	C10H10	000767-60-2	90

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Peak Number 6 Benzo[c]thiophene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.20	5.82 ug/l	98049	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[c]thiophene	134	C8H6S	000270-82-6	95
2	Benzo[b]thiophene	134	C8H6S	000095-15-8	93
3	Cyclopenta[c]thiapyran	134	C8H6S	000270-63-3	83
4	Benzo[b]cyclobuta[d]thiophene-1,...	278	C14H14O4S	057156-87-3	78
5	Benzo[b]cyclobuta[d]thiophene-1,...	264	C13H12O4S	034244-75-2	78

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Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.12	11.15 ug/l	187840	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual

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

1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	Benzocycloheptatriene	142	C11H10	000264-09-5	91
4	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59

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Peak Number 8 1H-Inden-1-one, 2,3-dihydro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.21	5.81 ug/l	97785	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	98
2	N-Ethylbenzimidoyl bromide	211	C9H10BrN	041182-87-0	80
3	Naphthalene, 1,2,3,4-tetrahydro-	132	C10H12	000119-64-2	64
4	Isoquinoline, 1,2,3,4-tetrahydro-	133	C9H11N	000091-21-4	64
5	2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	64

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Peak Number 9 Bicyclo[4.4.1]undeca-1,3,5,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.32	7.39 ug/l	124443	1,4-Dichlorobenzene-d4	13.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3	Bicyclo[4.4.1]undeca-1,3,5,7,9-p...	142	C11H10	002443-46-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	90

Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propane	1.80	38.0	ug/l	374420	1	7.63	492210	50.0
Acetic acid	8.27	5.3	ug/l	70640	2	8.55	671354	50.0
unknown13.43	13.43	7.7	ug/l	129358	4	13.32	842160	50.0
Indene	13.70	39.3	ug/l	661507	4	13.32	842160	50.0
2-Methylindene	14.64	5.5	ug/l	93325	4	13.32	842160	50.0
Benzo[c]thiophene	15.20	5.8	ug/l	98049	4	13.32	842160	50.0
Naphthalene, 1-me...	16.12	11.2	ug/l	187840	4	13.32	842160	50.0
1H-Inden-1-one, 2...	16.21	5.8	ug/l	97785	4	13.32	842160	50.0
Bicyclo[4.4.1]und...	16.32	7.4	ug/l	124443	4	13.32	842160	50.0