LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032419\
Data File : VN054645.D
Acq On : 24 Mar 2019 13:55
Operator : JC/SP
Sample : K2047-07
Misc : 6.74g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WP022SB445-190320-(17-19)

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\82N032019W.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	2.481	201	220	221	rBV5	27389	49633	1.72%	0.214%
2	2.519	226	232	233	rVV	43813	54986	1.91%	0.238%
3	2.555	235	243	260	rVB4	77864	148310	5.15%	0.641%
4	7.590	1792	1809	1819	rBV	341407	865439	30.06%	3.739%
5	7.661	1820	1831	1848	rVB	600819	1415864	49.17%	6.117%
6	7.866	1882	1895	1911	rVB5	28094	65817	2.29%	0.284%
7	8.024	1922	1944	1965	rBV	402563	941162	32.69%	4.066%
8	8.201	1988	1999	2019	rVB2	47661	127841	4.44%	0.552%
9	8.432	2061	2071	2080	rBV6	21015	41232	1.43%	0.178%
10	8.583	2102	2118	2156	rVB	920256	2009137	69.78%	8.680%
11	9.079	2255	2272	2284	rBV4	69231	163144	5.67%	0.705%
12	9.136	2284	2290	2302	rVB4	18274	36000	1.25%	0.156%
13	9.516	2396	2408	2423	rVB4	38551	83906	2.91%	0.362%
14	9.651	2436	2450	2463	rBV4	44372	103695	3.60%	0.448%
15	9.728	2463	2474	2496	rVB4	47658	122066	4.24%	0.527%
16	9.866	2502	2517	2537	rVB2	42439	107167	3.72%	0.463%
17	10.021	2555	2565	2573	rBV2	26871	45500	1.58%	0.197%
18	10.088	2573	2586	2619	rBV	1420829	2879441	100.00%	12.440%
19	10.429	2681	2692	2708	rVB4	21539	42094	1.46%	0.182%
20	10.718	2769	2782	2791	rBV5	27704	49531	1.72%	0.214%
21	10.818	2804	2813	2825	rBV	23346	46792	1.63%	0.202%
22	10.950	2846	2854	2862	rVB	31534	47332	1.64%	0.204%
23	11.004	2862	2871	2882	rVB3	33512	57889	2.01%	0.250%
24	11.123	2895	2908	2915	rBV5	28843	55047	1.91%	0.238%
25	11.194	2916	2930	2951	rVB5	63753	173369	6.02%	0.749%
26	11.297	2951	2962	2977	rBV	91351	163641	5.68%	0.707%
27	11.413	2983	2998	3000	rBV	1370999	2239422	77.77%	9.675%
28	11.593	3045	3054	3063	rBV9	17874	36640	1.27%	0.158%
29	11.654	3063	3073	3081	rBV5	55659	103913	3.61%	0.449%
30	11.853	3126	3135	3143	rBV4	48679	77893	2.71%	0.337%
31	11.927	3144	3158	3168	rBV6	108100	239319	8.31%	1.034%
32	12.043	3186	3194	3203	rVB	153843	224160	7.78%	0.968%
33	12.117	3208	3217	3222	rVV7	72489	129115	4.48%	0.558%
34	12.159	3223	3230	3241	rVB4	136679	247560	8.60%	1.070%

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Instrument : MSVOA_N
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Integration Parameters: RTEINT.P
Integrator: RTE
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Title : SW846 8260

35	12.297	3260	3273	3278	rBV6	103973	239475	8.32%	1.035%
36	12.336	3280	3285	3293	rVV	202314	276165	9.59%	1.193%
37	12.400	3294	3305	3326	rVB	986228	1766466	61.35%	7.631%
38	12.561	3348	3355	3370	rVB6	98569	207046	7.19%	0.894%
39	12.648	3370	3382	3392	rBV6	46505	134205	4.66%	0.580%
40	12.728	3394	3407	3416	rBV7	131577	300827	10.45%	1.300%
41	12.873	3444	3452	3460	rBV4	93411	190750	6.62%	0.824%
42	12.963	3473	3480	3491	rVB	391431	614640	21.35%	2.655%
43	13.024	3493	3499	3511	rVB4	97349	167284	5.81%	0.723%
44	13.088	3511	3519	3528	rBV3	136524	226016	7.85%	0.976%
45	13.143	3529	3536	3550	rVB6	115161	237430	8.25%	1.026%
46	13.239	3551	3566	3573	rBV5	248040	505307	17.55%	2.183%
47	13.284	3574	3580	3586	rVV3	199472	312224	10.84%	1.349%
48	13.342	3587	3598	3619	rVB	1152156	2265837	78.69%	9.789%
49	13.615	3671	3683	3685	rBV7	42790	82045	2.85%	0.354%
50	13.657	3687	3696	3707	rVV3	336575	647838	22.50%	2.799%
51	13.712	3708	3713	3721	rVV4	60171	98114	3.41%	0.424%
52	13.837	3743	3752	3761	rBV6	105925	225521	7.83%	0.974%
53	13.992	3792	3800	3809	rBV5	101948	164257	5.70%	0.710%
54	14.059	3811	3821	3831	rVB5	72673	152513	5.30%	0.659%
55	14.178	3849	3858	3877	rVB7	217626	560160	19.45%	2.420%
56	14.297	3888	3895	3900	rBV5	76388	111766	3.88%	0.483%
57	14.332	3901	3906	3915	rVB6	95079	127587	4.43%	0.551%
58	14.525	3962	3966	3974	rVB3	38147	43805	1.52%	0.189%
59	14.586	3979	3985	3994	rVV7	64928	129014	4.48%	0.557%
60	14.641	3997	4002	4014	rVB4	80218	122912	4.27%	0.531%
61	14.850	4061	4067	4074	rBV5	33100	43954	1.53%	0.190%

Sum of corrected areas: 23147215

LSC Report - Integrated Chromatogram

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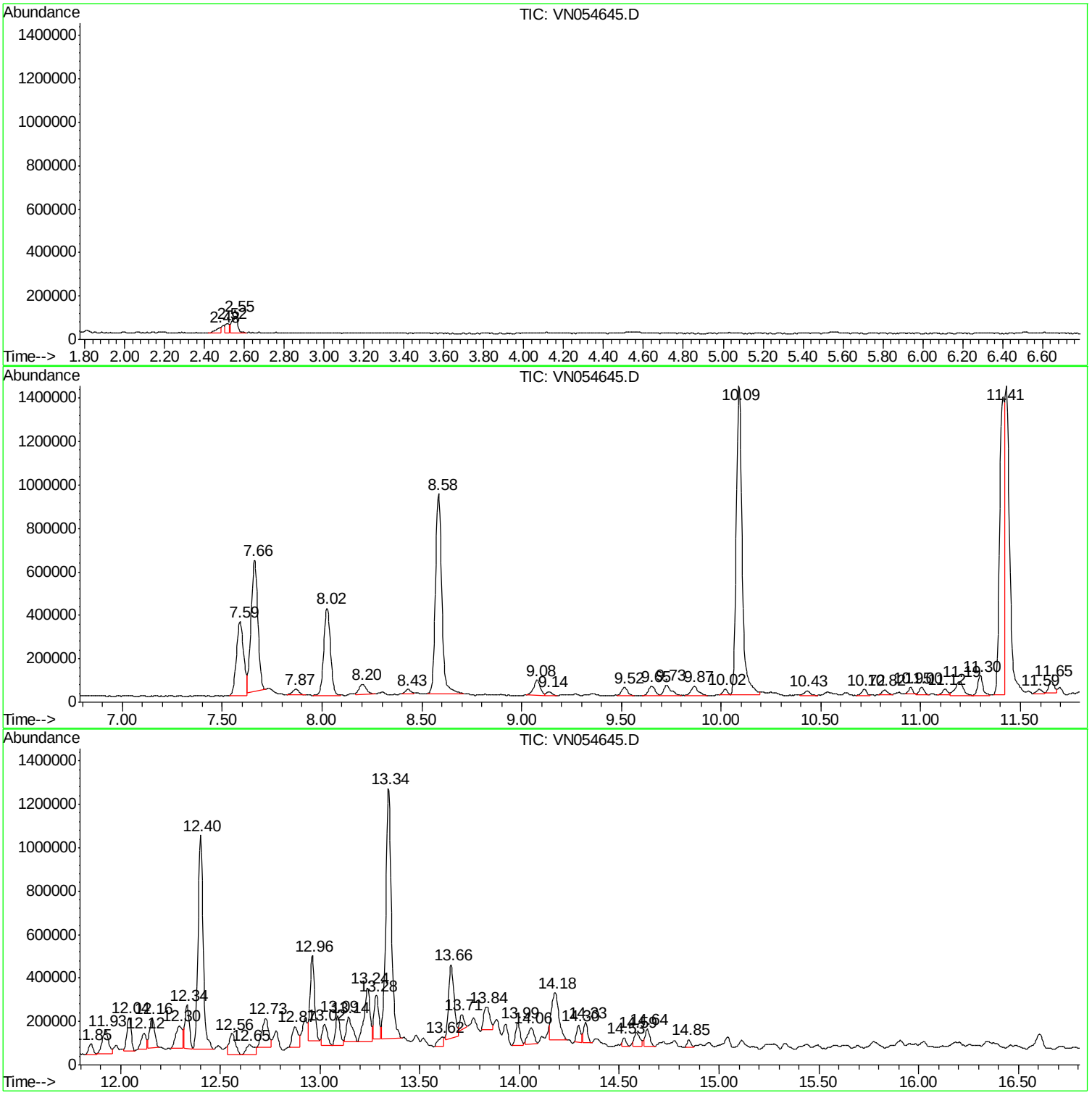
Instrument : MSVOA_N
ClientSampleId : WP022SB445-190320-(17-19)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.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\82N032019W.M
Quant Title : SW846 8260

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

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Peak Number 1 Octane, 3,5-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	5.34 ug/l	239319	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	60
2	Heptane, 2,3,4-trimethyl-	142	C10H22	052896-95-4	47
3	Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	38
4	Hexamethylenimine	99	C6H13N	000111-49-9	38
5	Octane, 2,5-dimethyl-	142	C10H22	015869-89-3	38

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Peak Number 2 Octane, 2,6-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.04	5.00 ug/l	224160	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	90
2	Octane, 3,6-dimethyl-	142	C10H22	015869-94-0	87
3	Nonane, 3-methyl-	142	C10H22	005911-04-6	86
4	Undecane, 6,6-dimethyl-	184	C13H28	017312-76-4	59
5	Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	53

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Peak Number 3 Cyclohexane, propyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.16	5.53 ug/l	247560	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, propyl-	126	C9H18	001678-92-8	68
2	Cyclohexane, methyl-	98	C7H14	000108-87-2	68
3	Cyclohexane, ethyl-	112	C8H16	001678-91-7	50
4	Cyclopropane, 1,1,2,2-tetramethyl-	98	C7H14	004127-47-3	49
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	49

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Peak Number 4 Heptane, 3,4,5-trimethyl- Concentration Rank 6

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

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ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WP022SB445-190320-(17-19)

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.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.
12.30	5.35 ug/l	239475	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3,4,5-trimethyl-	142	C10H22	020278-89-1	59
2	Undecane, 5,6-dimethyl-	184	C13H28	017615-91-7	59
3	Hexane, 2,4-dimethyl-	114	C8H18	000589-43-5	52
4	Octane, 2-methyl-	128	C9H20	003221-61-2	50
5	Heptane, 4-ethyl-	128	C9H20	002216-32-2	50

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Peak Number 5 Nonane, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.34	6.17 ug/l	276165	Chlorobenzene-d5	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane, 4-methyl-	142	C10H22	017301-94-9	64
2	Octane, 3,5-dimethyl-	142	C10H22	015869-93-9	64
3	Heptane, 2,3,4-trimethyl-	142	C10H22	052896-95-4	53
4	Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	50
5	5-Octadecenal	266	C18H34O	056554-88-2	47

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Peak Number 6 Cyclohexane, 1-methyl-2-pen... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	6.64 ug/l	300827	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 1-methyl-2-pentyl-	168	C12H24	054411-01-7	64
2	Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	59
3	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	006236-88-0	53
4	Oxalic acid, cyclohexylmethyl et...	214	C11H18O4	1000309-68-0	53
5	Cyclohexane, 1-ethyl-4-methyl-, ...	126	C9H18	004926-78-7	53

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Peak Number 7 Octane, 3,3-dimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.96	13.56 ug/l	614640	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual

Library Search Compound Report

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Instrument :
MSVOA_N
ClientSampleId :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N032019W.M
Quant Title : SW846 8260

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

1	Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	83
2	Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	78
3	Decane, 4-methyl-	156	C11H24	002847-72-5	72
4	Dodecane, 4-methyl-	184	C13H28	006117-97-1	64
5	Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	64

Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Octane, 3,5-dimet...	11.93	5.3	ug/l	239319	3	11.41	2239420	50.0
Octane, 2,6-dimet...	12.04	5.0	ug/l	224160	3	11.41	2239420	50.0
Cyclohexane, propyl-	12.16	5.5	ug/l	247560	3	11.41	2239420	50.0
Heptane, 3,4,5-tr...	12.30	5.3	ug/l	239475	3	11.41	2239420	50.0
Nonane, 4-methyl-	12.34	6.2	ug/l	276165	3	11.41	2239420	50.0
Cyclohexane, 1-me...	12.73	6.6	ug/l	300827	4	13.34	2265840	50.0
Octane, 3,3-dimet...	12.96	13.6	ug/l	614640	4	13.34	2265840	50.0