LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN032419\
Data File : VN054648.D
Acq On : 24 Mar 2019 15:15
Operator : JC/SP
Sample : K2047-10
Misc : 6.37g/5mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : WP022SB434-190320-(16-18)

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	2.555	238	243	263	rVB	98914	181199	5.12%	0.799%
2	7.590	1789	1809	1819	rBV	347348	858873	24.29%	3.787%
3	7.661	1820	1831	1852	rVB	621981	1474939	41.70%	6.503%
4	8.024	1926	1944	1972	rVB2	402860	949429	26.85%	4.186%
5	8.201	1980	1999	2016	rBV2	68949	184718	5.22%	0.814%
6	8.583	2102	2118	2165	rVB	935943	2088603	59.06%	9.209%
7	9.516	2395	2408	2421	rVB2	41775	84843	2.40%	0.374%
8	9.648	2435	2449	2464	rBV3	70101	149900	4.24%	0.661%
9	10.021	2556	2565	2573	rBV2	33073	58306	1.65%	0.257%
10	10.088	2573	2586	2624	rVB	1398029	2814483	79.58%	12.409%
11	11.410	2982	2997	3032	rBV2	1314105	3536632	100.00%	15.593%
12	11.599	3047	3056	3065	rBV4	27935	52516	1.48%	0.232%
13	11.660	3069	3075	3093	rVB5	33280	70214	1.99%	0.310%
14	11.760	3093	3106	3111	rBV9	18910	37063	1.05%	0.163%
15	11.905	3141	3151	3165	rBV5	58286	126945	3.59%	0.560%
16	11.979	3165	3174	3179	rBV5	46389	79867	2.26%	0.352%
17	12.043	3188	3194	3203	rVB2	65053	101964	2.88%	0.450%
18	12.123	3207	3219	3222	rBV10	63059	119937	3.39%	0.529%
19	12.217	3237	3248	3261	rBV7	92877	212797	6.02%	0.938%
20	12.339	3282	3286	3293	rVB3	40304	53643	1.52%	0.237%
21	12.403	3293	3306	3318	rBV	1062019	1857932	52.53%	8.192%
22	12.651	3369	3383	3394	rBV10	149762	451958	12.78%	1.993%
23	12.734	3396	3409	3413	rBV9	127915	315887	8.93%	1.393%
24	13.088	3512	3519	3533	rBV4	284015	575905	16.28%	2.539%
25	13.345	3589	3599	3613	rVB	1211046	2287161	64.67%	10.084%
26	13.657	3688	3696	3711	rVB9	385346	771513	21.81%	3.402%
27	14.043	3809	3816	3830	rVB8	205728	531133	15.02%	2.342%
28	14.168	3846	3855	3883	rBV2	640072	1971084	55.73%	8.691%
29	14.303	3891	3897	3901	rBV	182694	268356	7.59%	1.183%
30	14.898	4075	4082	4104	rBV9	160742	412942	11.68%	1.821%

Sum of corrected areas: 22680742

LSC Report - Integrated Chromatogram

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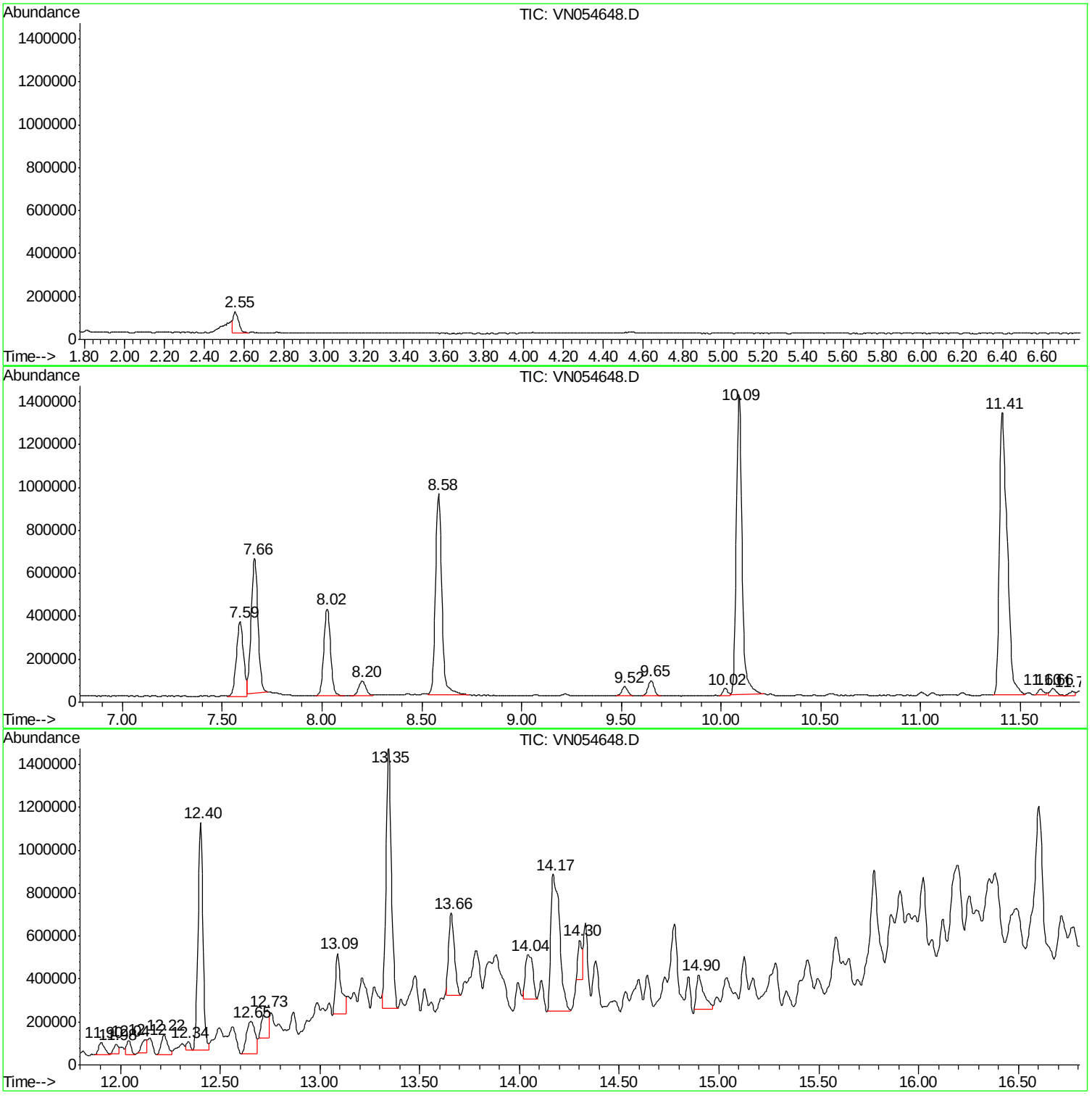
ClientSampleId :
WP022SB434-190320-(16-18)

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 unknown12.65 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	9.88 ug/l	451958	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, (1-methylethylidene)-	96	C7H12	001528-22-9	43
2	Furan, 2-ethyl-	96	C6H8O	003208-16-0	43
3	1-Methyl-4-(1-methylethyl)-cyclo...	140	C10H20	000099-82-1	38
4	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	38
5	Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	001678-82-6	38

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Peak Number 2 unknown12.73 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.73	6.91 ug/l	315887	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1R,2c,3t,4t-Tetramethyl-cyclohexane	140	C10H20	1000144-07-3	43
2	Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	38
3	1-Heptanol, 2,4-diethyl-	172	C11H24O	080192-55-8	35
4	Hexane, 3-methyl-	100	C7H16	000589-34-4	35
5	1-Hexanol, 5-methyl-2-(1-methyle...	158	C10H22O	002051-33-4	27

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Peak Number 3 Decane, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.09	12.59 ug/l	575905	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decane, 3-methyl-	156	C11H24	013151-34-3	81
2	Dodecane, 3-methyl-	184	C13H28	017312-57-1	72
3	Nonane, 3,7-dimethyl-	156	C11H24	017302-32-8	72
4	Heptacosane	380	C27H56	000593-49-7	64
5	Undecane, 3-methyl-	170	C12H26	001002-43-3	64

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Peak Number 4 Adamantane Concentration Rank 3

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

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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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	11.61 ug/l	531133	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adamantane	136	C10H16	000281-23-2	81
2	2,5-Methano-1H-indene, octahydro-	136	C10H16	019026-94-9	59
3	Bicyclo[3.3.1]non-2-en-9-one	136	C9H12O	004844-11-5	58
4	Tricyclo[5.2.1.0(4,8)]decane	136	C10H16	042836-61-3	53
5	Bicyclo[2.2.1]heptane, 2,2-dimet...	136	C10H16	000497-32-5	46

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Peak Number 5 trans-Decalin, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	43.09 ug/l	1971080	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	95
2	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	95
3	Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	83
4	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	76
5	Camphor	152	C10H16O	000076-22-2	62

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Peak Number 6 Pyridine, pentamethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.30	5.87 ug/l	268356	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine, pentamethyl-	149	C10H15N	003748-83-2	50
2	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	49
3	5H-Pyrrolo(3,2-d)pyrimidine-2,4-...	149	C6H7N5	1000244-21-4	42
4	Phthalic acid, isobutyl tridec-2...	400	C25H36O4	1000315-44-3	40
5	Pyridinium, 1-(acetylamino)-2,6-...	164	C9H12N2O	031020-35-6	38

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.90	9.03 ug/l	412942	1,4-Dichlorobenzene-d4	13.34

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual

Library Search Compound Report

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MSVOA_N
ClientSampleId :
WP022SB434-190320-(16-18)

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	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	90
2	1,4-Dimethyladamantane	164	C12H20	024145-89-9	49
3	2-(3-Methylbuta-1,3-dienyl)cyclo...	164	C11H16O	1000191-75-5	43
4	Pyridine, pentamethyl-	149	C10H15N	003748-83-2	43
5	Benzene, 2-methoxy-4-methyl-1-(1...	164	C11H16O	001076-56-8	43

Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown12.65	12.65	9.9	ug/l	451958	4	13.34	2287160	50.0
unknown12.73	12.73	6.9	ug/l	315887	4	13.34	2287160	50.0
Decane, 3-methyl-	13.09	12.6	ug/l	575905	4	13.34	2287160	50.0
Adamantane	14.04	11.6	ug/l	531133	4	13.34	2287160	50.0
trans-Decalin, 2-...	14.17	43.1	ug/l	1971080	4	13.34	2287160	50.0
Pyridine, pentame...	14.30	5.9	ug/l	268356	4	13.34	2287160	50.0
Adamantane, 1,3-d...	14.90	9.0	ug/l	412942	4	13.34	2287160	50.0