LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN020419\
Data File : VN053591.D
Acq On : 4 Feb 2019 12:49
Operator : JC/SP
Sample : K1299-01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 0035-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\82N013019W.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	2.471	201	217	218	rBV4	21515	38178	1.11%	0.165%
2	7.590	1789	1809	1820	rBV	445068	1111884	32.39%	4.818%
3	7.664	1820	1832	1890	rVB	684932	1817974	52.96%	7.877%
4	8.024	1927	1944	1973	rBV	418454	981206	28.58%	4.251%
5	8.583	2102	2118	2174	rVB	1062899	2441149	71.11%	10.577%
6	10.091	2570	2587	2631	rBV	1621408	3432947	100.00%	14.874%
7	11.005	2861	2871	2882	rVB3	22253	40542	1.18%	0.176%
8	11.120	2896	2907	2917	rBV4	18645	38141	1.11%	0.165%
9	11.210	2926	2935	2952	rVB4	17944	37514	1.09%	0.163%
10	11.406	2981	2996	3021	rBV	1481505	2841016	82.76%	12.310%
11	11.616	3045	3061	3066	rBV8	17641	47327	1.38%	0.205%
12	11.924	3143	3157	3172	rBV10	37260	122383	3.56%	0.530%
13	12.043	3186	3194	3203	rVB2	59252	85260	2.48%	0.369%
14	12.120	3209	3218	3222	rBV6	35688	58992	1.72%	0.256%
15	12.156	3223	3229	3241	rVB4	67237	123496	3.60%	0.535%
16	12.294	3267	3272	3282	rVB5	34623	56367	1.64%	0.244%
17	12.403	3293	3306	3322	rBV	1266562	2223333	64.76%	9.633%
18	12.561	3347	3355	3369	rVB7	63170	123476	3.60%	0.535%
19	12.654	3370	3384	3392	rBV4	86455	177376	5.17%	0.769%
20	12.731	3397	3408	3417	rVV6	89284	174061	5.07%	0.754%
21	12.876	3445	3453	3464	rBV5	35677	95181	2.77%	0.412%
22	12.963	3473	3480	3493	rVB	114407	196983	5.74%	0.853%
23	13.040	3494	3504	3512	rBV2	86631	151112	4.40%	0.655%
24	13.091	3514	3520	3529	rVB3	32603	47144	1.37%	0.204%
25	13.143	3530	3536	3551	rVB7	43055	96759	2.82%	0.419%
26	13.239	3552	3566	3575	rBV9	125584	310339	9.04%	1.345%
27	13.345	3587	3599	3618	rVB	1568389	2701796	78.70%	11.706%
28	13.583	3667	3673	3684	rBV2	46383	69579	2.03%	0.301%
29	13.664	3689	3698	3707	rVV7	108187	212603	6.19%	0.921%
30	13.712	3709	3713	3724	rVB6	52902	82127	2.39%	0.356%
31	13.995	3794	3801	3809	rVB3	63533	91510	2.67%	0.396%
32	14.172	3846	3856	3867	rBV3	136034	308366	8.98%	1.336%
33	14.332	3900	3906	3914	rVB4	90425	120977	3.52%	0.524%
34	14.590	3979	3986	3994	rVV5	115650	190338	5.54%	0.825%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN020419\
Data File : VN053591.D
Acq On : 4 Feb 2019 12:49
Operator : JC/SP
Sample : K1299-01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 0035-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\82N013019W.M
Title : SW846 8260

35	14.641	3995	4002	4015	rVB4	199461	346928	10.11%	1.503%
36	15.130	4142	4154	4175	rVB2	391293	876541	25.53%	3.798%
37	16.033	4429	4435	4447	rVB3	94499	155942	4.54%	0.676%
38	16.159	4465	4474	4498	rVB	207237	432808	12.61%	1.875%
39	16.352	4523	4534	4557	rVB	253470	620209	18.07%	2.687%

Sum of corrected areas: 23079864

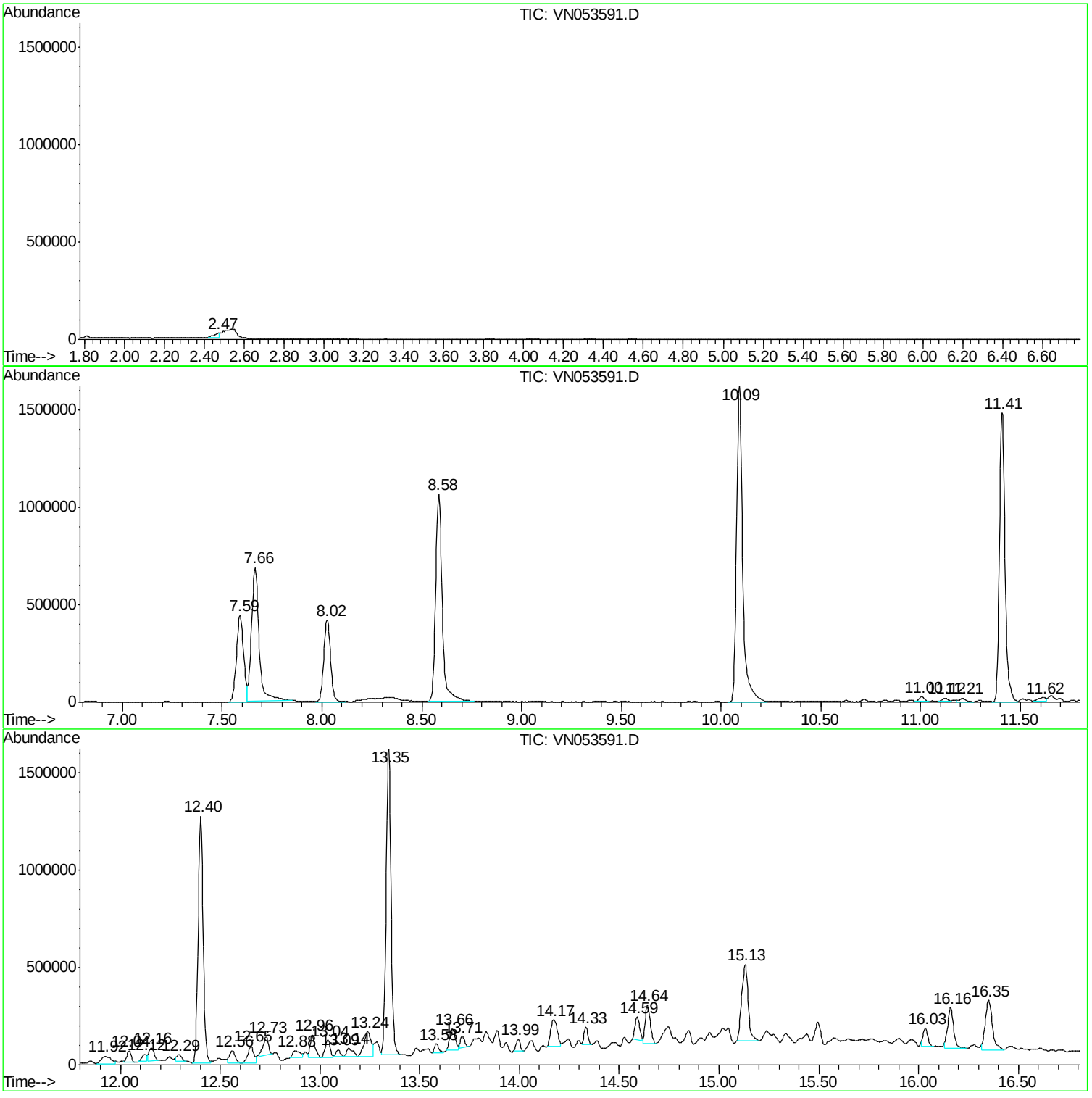
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN020419\
Data File : VN053591.D
Acq On : 4 Feb 2019 12:49
Operator : JC/SP
Sample : K1299-01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 0035-COMP-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N013019W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN020419\
Data File : VN053591.D
Acq On : 4 Feb 2019 12:49
Operator : JC/SP
Sample : K1299-01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 0035-COMP-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N013019W.M
Quant Title : SW846 8260

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

****

Peak Number 1 Cyclohexane, (2-methylpropyl)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.24	5.74 ug/l	310339	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	58
2	Cyclohexane, butyl-	140	C10H20	001678-93-9	52
3	Cyclohexane, (1-methylethyl)-	126	C9H18	000696-29-7	49
4	Ethanone, 1-cyclohexyl-	126	C8H14O	000823-76-7	45
5	Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	43

****

Peak Number 2 Cyclohexane, pentyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.17	5.71 ug/l	308366	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, pentyl-	154	C11H22	004292-92-6	49
2	1-Pentadecyne	208	C15H28	000765-13-9	46
3	Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	46
4	Decalin, anti-1-methyl-, cis-	152	C11H20	1000158-89-0	45
5	Cyclohexane, 2-propenyl-	124	C9H16	002114-42-3	43

****

Peak Number 3 Undecane, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.64	6.42 ug/l	346928	1,4-Dichlorobenzene-d4	13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	60
2	Undecane, 3,6-dimethyl-	184	C13H28	017301-28-9	46
3	Heptane, 3-(bromomethyl)-	192	C8H17Br	018908-66-2	43
4	Tridecane, 7-methyl-	198	C14H30	026730-14-3	38
5	Nonane, 3-methyl-	142	C10H22	005911-04-6	30

****

Peak Number 4 Naphthalene, 1-methyl- Concentration Rank 2

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

Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN020419\
Data File : VN053591.D
Acq On : 4 Feb 2019 12:49
Operator : JC/SP
Sample : K1299-01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 0035-COMP-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N013019W.M
Quant Title : SW846 8260

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

16.16 8.01 ug/l 432808 1,4-Dichlorobenzene-d4 13.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4	Benzocycloheptatriene	142	C11H10	000264-09-5	91
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	87

Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_N\DATA\VN020419\
Data File : VN053591.D
Acq On : 4 Feb 2019 12:49
Operator : JC/SP
Sample : K1299-01
Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
ALS Vial : 7 Sample Multiplier: 28

Instrument : MSVOA_N
ClientSampleId : 0035-COMP-1

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_N\METHODS\82N013019W.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
Cyclohexane, (2-m...	13.24	5.7	ug/l	310339	4	13.35	2701800	50.0
Cyclohexane, pentyl-	14.17	5.7	ug/l	308366	4	13.35	2701800	50.0
Undecane, 2,6-dim...	14.64	6.4	ug/l	346928	4	13.35	2701800	50.0
Naphthalene, 1-me...	16.16	8.0	ug/l	432808	4	13.35	2701800	50.0