LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX081919\
Data File : VX011626.D
Acq On : 19 Aug 2019 12:58
Operator : JC/SP
Sample : K4351-01
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : PH2-0142

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_X\METHOD\82X081519W.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	1.398	36	40	65	rVV	12084164	13643606	7.15%	2.614%
2	1.782	98	103	119	rVB	2832651	3810668	2.00%	0.730%
3	1.995	132	138	152	rVB	5726624	8511460	4.46%	1.631%
4	2.928	286	291	306	rVB	1368524	2909617	1.53%	0.557%
5	3.519	378	388	403	rBV	961659	2155294	1.13%	0.413%
6	4.397	520	532	547	rVB	3806092	11015837	5.78%	2.111%
7	5.580	715	726	736	rBV	6776956	20623861	10.81%	3.952%
8	5.933	768	784	796	rBV4	556655	1928169	1.01%	0.369%
9	6.452	861	869	883	rVB	1009220	2754217	1.44%	0.528%
10	7.464	1022	1035	1046	rBV	9877539	22389145	11.74%	4.290%
11	8.713	1235	1240	1245	rVB	1204448	2132920	1.12%	0.409%
12	8.787	1245	1252	1257	rBV	17022237	26628141	13.96%	5.102%
13	10.262	1486	1494	1499	rBV2	45370332	74296391	38.96%	14.235%
14	10.390	1502	1515	1520	rBV3	79385470	190702016	100.00%	36.539%
15	10.701	1560	1566	1572	rVB	26452112	36916945	19.36%	7.073%
16	11.018	1612	1618	1627	rVB	5844606	7422967	3.89%	1.422%
17	11.359	1669	1674	1680	rVV	4996686	6059678	3.18%	1.161%
18	11.432	1680	1686	1694	rVV	14725618	26102486	13.69%	5.001%
19	11.506	1694	1698	1704	rVB	8309010	9738124	5.11%	1.866%
20	11.664	1716	1724	1730	rBV	7392578	9285210	4.87%	1.779%
21	11.810	1742	1748	1753	rVB	19207661	24277611	12.73%	4.652%
22	12.073	1786	1791	1797	rVV2	1377225	2053138	1.08%	0.393%
23	12.140	1797	1802	1807	rVB	7680187	9237115	4.84%	1.770%
24	12.298	1821	1828	1835	rBV2	1998289	3101734	1.63%	0.594%
25	13.828	2072	2079	2087	rVB	3292907	4219799	2.21%	0.809%

Sum of corrected areas: 521916149

LSC Report - Integrated Chromatogram

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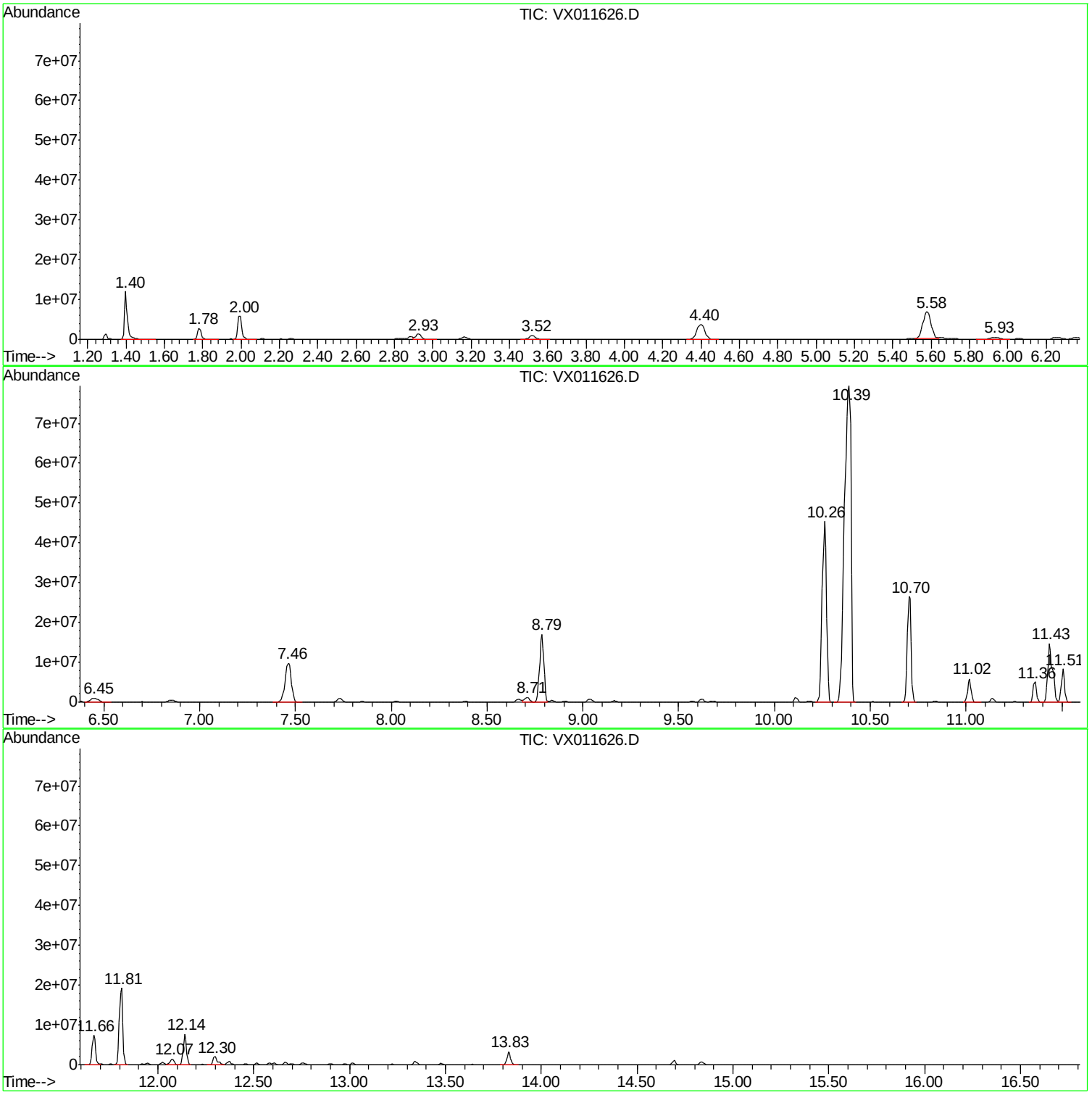
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081519W.M
Quant Title : SW846 8260

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



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Peak Number 1 Butane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.40	33.08 ug/l	13643600	Pentafluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	80
2	Isobutane	58	C4H10	000075-28-5	9
3	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9
5	Diazene, dimethyl-	58	C2H6N2	000503-28-6	4

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Peak Number 2 Butane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.78	9.24 ug/l	3810670	Pentafluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2	3-Buten-1-ol	72	C4H8O	000627-27-0	47
3	Pentane	72	C5H12	000109-66-0	36
4	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	30
5	Azetidine	57	C3H7N	000503-29-7	9

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Peak Number 3 Pentane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	20.64 ug/l	8511460	Pentafluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Butane, 2-methyl-	72	C5H12	000078-78-4	38
3	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	35
4	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	9
5	Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	9

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Peak Number 4 Cyclopentane Concentration Rank 10

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

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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : PH2-0142

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081519W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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2.93	7.05 ug/l	2909620	Pentafluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	78
2	1-Pentene	70	C5H10	000109-67-1	39
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	9
4	Carbonochloridic acid, pentyl ester	150	C6H11ClO2	000638-41-5	9
5	Methyl propargyl ether	70	C4H6O	000627-41-8	7

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Peak Number 5 Cyclopentane, methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	26.71 ug/l	11015800	Pentafluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	64

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Peak Number 6 Cyclopentane, 1,2-dimethyl-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.45	50.00 ug/l	2754220	1,4-Difluorobenzene	6.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	94
2	Isopropylcyclobutane	98	C7H14	000872-56-0	94
3	Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	91
4	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	90
5	Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	90

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Peak Number 7 Benzene, 1-ethyl-3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	635.67 ug/l	26102500	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual

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Instrument : MSVOA_X
ClientSampleId : PH2-0142

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081519W.M
Quant Title : SW846 8260

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

1	Benzene, 1-ethyl-3-methyl-	120 C9H12	000620-14-4	97
2	Benzene, 1-ethyl-2-methyl-	120 C9H12	000611-14-3	95
3	Mesitylene	120 C9H12	000108-67-8	91
4	Benzene, 1,2,4-trimethyl-	120 C9H12	000095-63-6	91
5	Benzene, 1,2,3-trimethyl-	120 C9H12	000526-73-8	91

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Peak Number 8 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	226.12 ug/l	9285210	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91

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Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.14	224.95 ug/l	9237120	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Mesitylene	120	C9H12	000108-67-8	91

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Peak Number 10 Indane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	75.54 ug/l	3101730	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	76
2	Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	68

Library Search Compound Report

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Instrument :
MSVOA_X
ClientSampleId :
PH2-0142

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X081519W.M
Quant Title : SW846 8260

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

4	Deltacyclene	118	C9H10	007785-10-6	58
5	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	55

Tentatively Identified Compound (LSC) summary

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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
Butane	1.40	33.1	ug/l	13643600	1	5.66	20623900	50.0
Butane, 2-methyl-	1.78	9.2	ug/l	3810670	1	5.66	20623900	50.0
Pentane	2.00	20.6	ug/l	8511460	1	5.66	20623900	50.0
Cyclopentane	2.93	7.0	ug/l	2909620	1	5.66	20623900	50.0
Cyclopentane, met...	4.40	26.7	ug/l	11015800	1	5.66	20623900	50.0
Cyclopentane, 1,2...	6.45	50.0	ug/l	2754220	2	6.85	2754220	50.0
Benzene, 1-ethyl-...	11.43	635.7	ug/l	26102500	4	12.08	2053140	50.0
Benzene, 1-ethyl-...	11.66	226.1	ug/l	9285210	4	12.08	2053140	50.0
Benzene, 1,2,3-tr...	12.14	224.9	ug/l	9237120	4	12.08	2053140	50.0
Indane	12.30	75.5	ug/l	3101730	4	12.08	2053140	50.0