LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX032419\
Data File : VX008393.D
Acq On : 24 Mar 2019 15:42
Operator : JC/SP
Sample : K2059-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-7

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\82X032319W.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	1.276	16	20	34	rBV	265794	591576	32.46%	4.243%
2	1.404	38	41	45	rVV	95914	105493	5.79%	0.757%
3	1.788	99	104	114	rVB	444138	637841	35.00%	4.575%
4	2.001	134	139	150	rVB2	123439	216081	11.86%	1.550%
5	2.263	177	182	192	rVB	221105	350491	19.23%	2.514%
6	2.391	197	203	208	rVV	19078	37786	2.07%	0.271%
7	2.605	233	238	246	rBV	14983	27071	1.49%	0.194%
8	2.818	264	273	274	rBV2	37930	68024	3.73%	0.488%
9	2.891	281	285	288	rBV	45282	83215	4.57%	0.597%
10	2.934	288	292	304	rVB	106928	231059	12.68%	1.657%
11	3.172	323	331	344	rVB2	66823	165513	9.08%	1.187%
12	3.397	358	368	377	rBV4	7770	22955	1.26%	0.165%
13	3.525	380	389	400	rVV3	18549	44752	2.46%	0.321%
14	3.818	424	437	445	rBV	46109	117201	6.43%	0.841%
15	3.928	445	455	463	rVV	30030	80406	4.41%	0.577%
16	4.202	487	500	509	rBV3	31791	91474	5.02%	0.656%
17	4.403	524	533	544	rVB2	87119	254849	13.98%	1.828%
18	4.531	545	554	566	rVB4	19698	61808	3.39%	0.443%
19	5.305	671	681	697	rVB2	40980	130989	7.19%	0.940%
20	5.501	701	713	721	rBV	140499	409945	22.49%	2.941%
21	5.580	721	726	731	rVV2	34742	102054	5.60%	0.732%
22	5.665	731	740	766	rVB	237164	752422	41.28%	5.397%
23	5.933	774	784	795	rVB4	12408	39948	2.19%	0.287%
24	6.061	795	805	811	rBV	171966	450055	24.69%	3.228%
25	6.141	811	818	833	rVB	705214	1822661	100.00%	13.074%
26	6.305	833	845	848	rBV2	26005	77046	4.23%	0.553%
27	6.464	862	871	881	rVB2	18729	58567	3.21%	0.420%
28	6.860	925	936	944	rBV	389292	940815	51.62%	6.749%
29	7.256	994	1001	1009	rVB3	27454	61710	3.39%	0.443%
30	7.457	1025	1034	1042	rBV6	35678	98414	5.40%	0.706%
31	7.939	1105	1113	1114	rBV5	11370	22498	1.23%	0.161%
32	8.055	1123	1132	1139	rVB2	14034	35192	1.93%	0.252%
33	8.177	1143	1152	1154	rBV2	21973	42292	2.32%	0.303%
34	8.213	1154	1158	1163	rVV	51685	89810	4.93%	0.644%

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Title : SW846 8260

35	8.488	1194	1203	1210	rBV3	10825	26042	1.43%	0.187%
36	8.567	1210	1216	1224	rVB	40155	71717	3.93%	0.514%
37	8.713	1234	1240	1247	rBV	819229	1256275	68.93%	9.011%
38	8.780	1247	1251	1258	rVB	65683	106326	5.83%	0.763%
39	8.902	1264	1271	1276	rBV3	14330	27025	1.48%	0.194%
40	9.219	1318	1323	1333	rVB	26097	45532	2.50%	0.327%
41	9.518	1363	1372	1376	rVV3	16128	36155	1.98%	0.259%
42	9.567	1376	1380	1385	rVV5	7904	18634	1.02%	0.134%
43	9.817	1415	1421	1429	rBV7	8974	19101	1.05%	0.137%
44	10.012	1445	1453	1459	rBV6	9495	22219	1.22%	0.159%
45	10.109	1464	1469	1475	rBV	745153	1014163	55.64%	7.275%
46	10.250	1488	1492	1497	rVV	112502	145988	8.01%	1.047%
47	10.353	1504	1509	1515	rVB	135420	194262	10.66%	1.393%
48	11.018	1612	1618	1623	rVB	124642	160668	8.82%	1.152%
49	11.134	1632	1637	1643	rBV	616950	769706	42.23%	5.521%
50	11.359	1664	1674	1681	rVV	76492	110314	6.05%	0.791%
51	11.451	1684	1689	1694	rVV2	14656	24822	1.36%	0.178%
52	11.664	1719	1724	1732	rBV	59245	80500	4.42%	0.577%
53	12.079	1786	1792	1798	rBV	692504	893866	49.04%	6.412%
54	12.140	1798	1802	1806	rBV	20192	25740	1.41%	0.185%
55	12.298	1820	1828	1833	rBV	223074	279613	15.34%	2.006%
56	12.664	1883	1888	1892	rBV	50644	65009	3.57%	0.466%
57	12.755	1899	1903	1910	rVB2	44262	63792	3.50%	0.458%
58	12.975	1932	1939	1943	rBV	34665	49223	2.70%	0.353%
59	13.225	1976	1980	1987	rVB	28974	38884	2.13%	0.279%
60	13.347	1995	2000	2005	rVB2	51862	73314	4.02%	0.526%

Sum of corrected areas: 13940903

LSC Report - Integrated Chromatogram

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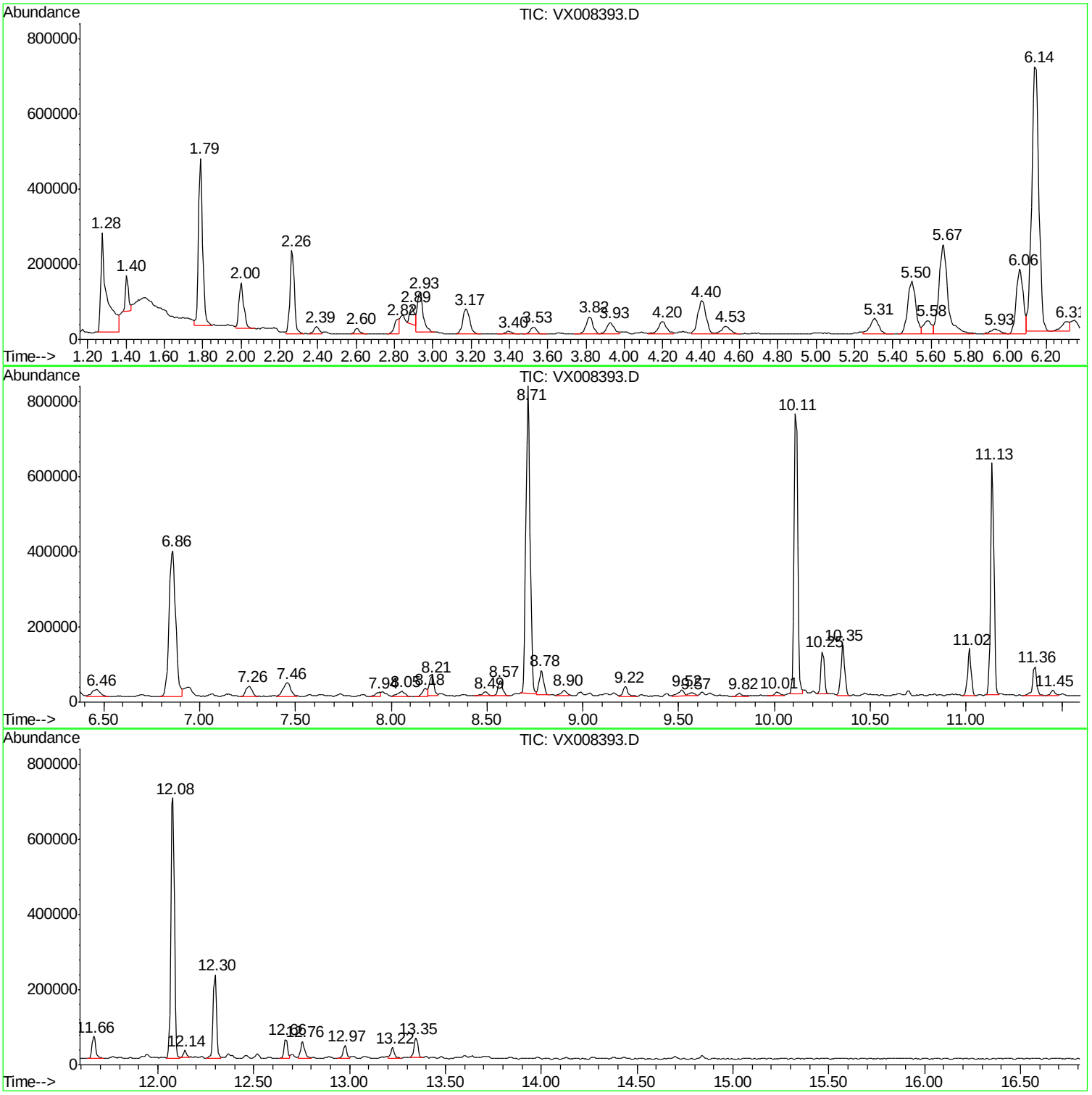
Sample : K2059-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032319W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX032419\
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ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032319W.M
Quant Title : SW846 8260

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

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Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.28	39.31 ug/l	591576	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3

****

Peak Number 2 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	42.39 ug/l	637841	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2	Pentane	72	C5H12	000109-66-0	36
3	3-Buten-1-ol	72	C4H8O	000627-27-0	28
4	1-Butene	56	C4H8	000106-98-9	10
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	9

****

Peak Number 3 Pentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	14.36 ug/l	216081	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	32
3	Tetrahydrofuran	72	C4H8O	000109-99-9	9
4	Propanal, 2-methyl-	72	C4H8O	000078-84-2	9
5	Butane, 2-methyl-	72	C5H12	000078-78-4	9

****

Peak Number 4 2-Butene, 2-methyl- Concentration Rank 3

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

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Sample : K2059-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032319W.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.
2.26	23.29 ug/l	350491	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 2-methyl-	70	C5H10	000513-35-9	91
2	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
3	2-Pentene, (E)-	70	C5H10	000646-04-8	87
4	2-Methyl-1-butene	70	C5H10	000563-46-2	86
5	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	83

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Peak Number 5 1-Pentene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.93	15.35 ug/l	231059	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	80
2	Cyclopentane	70	C5H10	000287-92-3	72
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	72
4	Cyclopropane, ethyl-	70	C5H10	001191-96-4	45
5	2H-Tetrazole, 2,5-dimethyl-	98	C3H6N4	004135-93-7	39

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Peak Number 6 Pentane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	11.00 ug/l	165513	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	87
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	56
3	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	56
4	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	56
5	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	53

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Peak Number 7 2-Butene, 2,3-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.82	7.79 ug/l	117201	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual

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ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : MW-7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X032319W.M
Quant Title : SW846 8260

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

1	2-Butene, 2,3-dimethyl-	84	C6H12	000563-79-1	91
2	Cyclopropane, 1,1,2-trimethyl-	84	C6H12	004127-45-1	91
3	2-Pentene, 2-methyl-	84	C6H12	000625-27-4	91
4	2-Pentene, 4-methyl-, (Z)-	84	C6H12	000691-38-3	91
5	2-Pentene, 4-methyl-	84	C6H12	004461-48-7	91

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Peak Number 8 Cyclopentane, methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	16.94 ug/l	254849	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclohexane	84	C6H12	000110-82-7	78
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	56
5	Cyclobutane, butyl-	112	C8H16	013152-44-8	45

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Peak Number 9 Cyclopentene, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.31	8.70 ug/l	130989	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene, 3-methyl-	82	C6H10	001120-62-3	90
2	Cyclopentene, 1-methyl-	82	C6H10	000693-89-0	87
3	Cyclopentene, 4-methyl-	82	C6H10	001759-81-5	86
4	Cyclohexene	82	C6H10	000110-83-8	83
5	1,4-Hexadiene, (Z)-	82	C6H10	007318-67-4	80

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Peak Number 10 Indane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	15.64 ug/l	279613	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	95
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	81
3	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	68

Library Search Compound Report

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TIC Integration Parameters: LSCINT.P

4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	58
5	Deltacyclene	118	C9H10	007785-10-6	58

Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	1.28	39.3	ug/l	591576	1	5.67	752422	50.0
Butane, 2-methyl-	1.79	42.4	ug/l	637841	1	5.67	752422	50.0
Pentane	2.00	14.4	ug/l	216081	1	5.67	752422	50.0
2-Butene, 2-methyl-	2.26	23.3	ug/l	350491	1	5.67	752422	50.0
1-Pentene	2.93	15.4	ug/l	231059	1	5.67	752422	50.0
Pentane, 3-methyl-	3.17	11.0	ug/l	165513	1	5.67	752422	50.0
2-Butene, 2,3-dim...	3.82	7.8	ug/l	117201	1	5.67	752422	50.0
Cyclopentane, met...	4.40	16.9	ug/l	254849	1	5.67	752422	50.0
Cyclopentene, 3-m...	5.31	8.7	ug/l	130989	1	5.67	752422	50.0
Indane	12.30	15.6	ug/l	279613	4	12.08	893866	50.0