LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX061418\
Data File : VX002551.D
Acq On : 14 Jun 2018 15:00
Operator : JC/MD
Sample : J3404-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SS050MW513-180607

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\82X060418W.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	1.075	76	80	93	rBV	2569354	3154922	100.00%	21.623%
2	1.489	144	148	157	rVB	33079	39886	1.26%	0.273%
3	2.002	227	232	240	rVB	23140	34323	1.09%	0.235%
4	2.447	299	305	317	rBV	74339	134727	4.27%	0.923%
5	4.355	609	618	629	rBV3	11032	32831	1.04%	0.225%
6	4.605	647	659	667	rBV	52253	148427	4.70%	1.017%
7	4.708	667	676	702	rVB	150617	460767	14.60%	3.158%
8	5.196	744	756	769	rBV2	33814	111473	3.53%	0.764%
9	5.507	796	807	821	rBV	178217	506324	16.05%	3.470%
10	5.665	821	833	850	rVB	263943	745793	23.64%	5.111%
11	6.074	889	900	917	rBV	203118	536269	17.00%	3.675%
12	6.867	1020	1030	1047	rBV	378230	893989	28.34%	6.127%
13	7.220	1079	1088	1104	rBV4	40060	121110	3.84%	0.830%
14	7.561	1137	1144	1155	rVB	65894	129045	4.09%	0.884%
15	7.732	1166	1172	1184	rVB	234201	419394	13.29%	2.874%
16	8.000	1206	1216	1227	rBV3	40020	105813	3.35%	0.725%
17	8.653	1318	1323	1328	rBV	25779	41448	1.31%	0.284%
18	8.720	1328	1334	1341	rVB	1019720	1528181	48.44%	10.474%
19	9.311	1425	1431	1437	rBV	23216	39013	1.24%	0.267%
20	9.378	1438	1442	1452	rVB	22437	32940	1.04%	0.226%
21	9.586	1468	1476	1490	rVB	97150	140041	4.44%	0.960%
22	10.116	1554	1563	1573	rBV	832477	1108834	35.15%	7.600%
23	10.640	1644	1649	1656	rBV	116665	161146	5.11%	1.104%
24	10.829	1673	1680	1686	rBV	83785	108829	3.45%	0.746%
25	10.939	1691	1698	1706	rVB	58032	92021	2.92%	0.631%
26	11.140	1726	1731	1742	rVB	898683	1140665	36.16%	7.818%
27	11.634	1806	1812	1817	rBV2	57598	105199	3.33%	0.721%
28	11.713	1822	1825	1829	rVV	28313	35351	1.12%	0.242%
29	11.780	1829	1836	1838	rVV4	36939	62283	1.97%	0.427%
30	11.817	1838	1842	1847	rVV	266386	318431	10.09%	2.182%
31	11.902	1851	1856	1862	rVV2	200223	312073	9.89%	2.139%
32	11.957	1862	1865	1875	rVB	151991	201898	6.40%	1.384%
33	12.079	1880	1885	1893	rVB	993170	1267363	40.17%	8.686%
34	12.640	1970	1977	1990	rBV2	59949	110270	3.50%	0.756%

LSC Area Percent Report

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ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SS050MW513-180607

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

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Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X060418W.M
Title : SW846 8260

35	12.750	1991	1995	2001	rVB4	22000	34166	1.08%	0.234%
36	12.829	2003	2008	2010	rBV	53173	71761	2.27%	0.492%
37	12.853	2010	2012	2020	rVB	84213	103822	3.29%	0.712%

Sum of corrected areas: 14590828

LSC Report - Integrated Chromatogram

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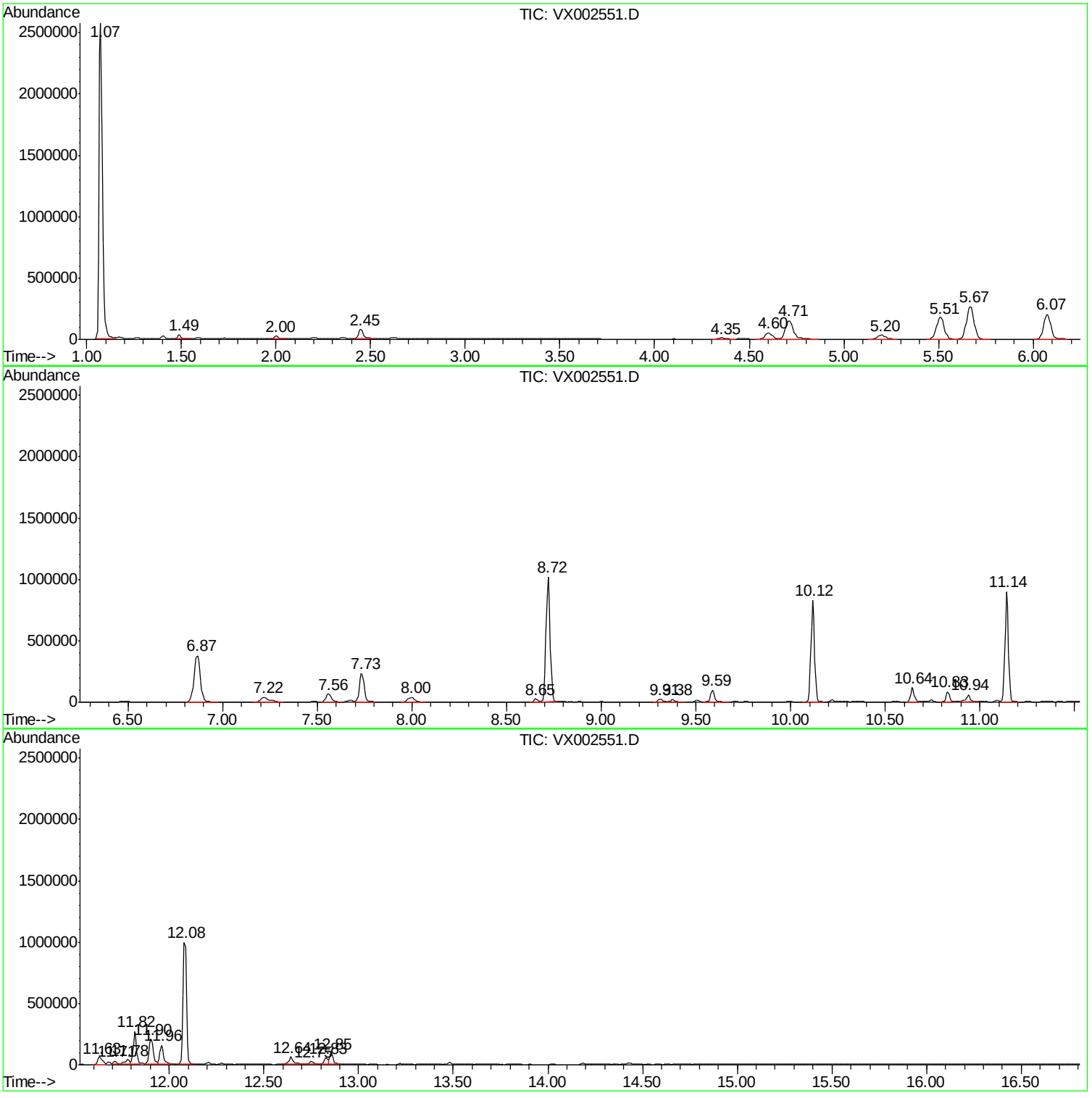
Instrument :
MSVOA_X
ClientSampleId :
SS050MW513-180607

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X060418W.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_X\METHOD\82X060418W.M
Quant Title : SW846 8260

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

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Peak Number 1 2-Pentanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	7.22 ug/l	129045	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone	86	C5H10O	000107-87-9	91
2	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	72
3	2,3-Butanedione	86	C4H6O2	000431-03-8	47
4	Ethanone, 1-oxiranyl-	86	C4H6O2	004401-11-0	9
5	2-Pentanone, 3-ethyl-	114	C7H14O	006137-03-7	9

****

Peak Number 2 3-Pentanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.73	23.46 ug/l	419394	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone	86	C5H10O	000096-22-0	90
2	Neopentane	72	C5H12	000463-82-1	9
3	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	7
4	Ethyl-1-propenyl ether	86	C5H10O	000928-55-2	7
5	Azetidine, 1-nitroso-	86	C3H6N2O	015216-10-1	5

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Peak Number 3 2-Butanol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.00	5.92 ug/l	105813	1,4-Difluorobenzene	6.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanol	74	C4H10O	000078-92-2	56
2	2-Heptanol	116	C7H16O	000543-49-7	53
3	(R)-(-)-2-Pentanol	88	C5H12O	031087-44-2	53
4	2-Pentanol	88	C5H12O	006032-29-7	42
5	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	42

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Peak Number 4 Hexanal Concentration Rank 8

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

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Acq On : 14 Jun 2018 15:00
Operator : JC/MD
Sample : J3404-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SS050MW513-180607

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X060418W.M
Quant Title : SW846 8260

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

9.59	6.31 ug/l	140041	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	64
2	Butanal	72	C4H8O	000123-72-8	43
3	2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	25
4	Butanal, 3-methyl-	86	C5H10O	000590-86-3	23
5	1-Butanol	74	C4H10O	000071-36-3	22

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Peak Number 5 1-Hexanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	7.27 ug/l	161146	Chlorobenzene-d5	10.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol	102	C6H14O	000111-27-3	83
2	Hexyl chloroformate	164	C7H13ClO2	006092-54-2	78
3	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	64
4	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	59
5	Cyclohexane	84	C6H12	000110-82-7	58

****

Peak Number 6 3-Octanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	12.56 ug/l	318431	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanone	128	C8H16O	000106-68-3	94
2	Ethanone, 1-(3,3-dimethyloxiranyl)-	114	C6H10O2	004478-63-1	50
3	Butanal, 2-ethyl-	100	C6H12O	000097-96-1	47
4	n-Caproic acid vinyl ester	142	C8H14O2	003050-69-9	47
5	3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	45

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Peak Number 7 2-Octanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.90	12.31 ug/l	312073	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual

Library Search Compound Report

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Sample : J3404-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 6 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : SS050MW513-180607

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X060418W.M
Quant Title : SW846 8260

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

1	2-Octanone	128	C8H16O	000111-13-7	52
2	2-Heptanone, 4-methyl-	128	C8H16O	006137-06-0	50
3	2-Heptanone	114	C7H14O	000110-43-0	47
4	2-Hexanone, 4-methyl-	114	C7H14O	000105-42-0	47
5	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	43

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Peak Number 8 2-Octanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.96	7.97 ug/l	201898	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanol	130	C8H18O	000123-96-6	90
2	2-Octanol, (R)-	130	C8H18O	005978-70-1	86
3	2-Octanol, (S)-	130	C8H18O	006169-06-8	86
4	2-Hexanol	102	C6H14O	000626-93-7	72
5	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	72

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
2-Pentanone	7.56	7.2	ug/l	129045	2	6.87	893989	50.0
3-Pentanone	7.73	23.5	ug/l	419394	2	6.87	893989	50.0
2-Butanol	8.00	5.9	ug/l	105813	2	6.87	893989	50.0
Hexanal	9.59	6.3	ug/l	140041	3	10.12	1108830	50.0
1-Hexanol	10.64	7.3	ug/l	161146	3	10.12	1108830	50.0
3-Octanone	11.82	12.6	ug/l	318431	4	12.09	1267360	50.0
2-Octanone	11.90	12.3	ug/l	312073	4	12.09	1267360	50.0
2-Octanol	11.96	8.0	ug/l	201898	4	12.09	1267360	50.0