LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112119\
Data File : VX013501.D
Acq On : 21 Nov 2019 14:27
Operator : JC/SP
Sample : K5967-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FERMENTATION-WASTE

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\82X103119W.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	1.070	26	30	42	rBV	6599120	8145419	100.00%	28.563%
2	1.320	65	71	79	rBV	86183	328917	4.04%	1.153%
3	2.430	248	253	262	rBV	63325	104546	1.28%	0.367%
4	2.698	291	297	304	rBV	60102	115823	1.42%	0.406%
5	2.850	316	322	331	rVB	93350	189079	2.32%	0.663%
6	4.661	612	619	630	rVB	62137	171511	2.11%	0.601%
7	5.112	684	693	707	rBV	230574	687689	8.44%	2.411%
8	5.490	742	755	768	rBV	410492	1158976	14.23%	4.064%
9	5.655	771	782	795	rVV	673850	1888403	23.18%	6.622%
10	6.051	836	847	861	rBV	462930	1168153	14.34%	4.096%
11	6.849	967	978	990	rBV	1098249	2561972	31.45%	8.984%
12	8.642	1263	1272	1277	rBV	54781	98923	1.21%	0.347%
13	8.709	1277	1283	1290	rVV	2338319	3570299	43.83%	12.520%
14	8.782	1290	1295	1298	rVV	75515	122985	1.51%	0.431%
15	8.825	1298	1302	1313	rVB2	65548	113222	1.39%	0.397%
16	10.105	1504	1512	1522	rBV	2170690	3003476	36.87%	10.532%
17	11.135	1675	1681	1689	rBV	1832346	2311247	28.37%	8.105%
18	12.074	1830	1835	1842	rVB	2319327	2777204	34.10%	9.738%

Sum of corrected areas: 28517844

LSC Report - Integrated Chromatogram

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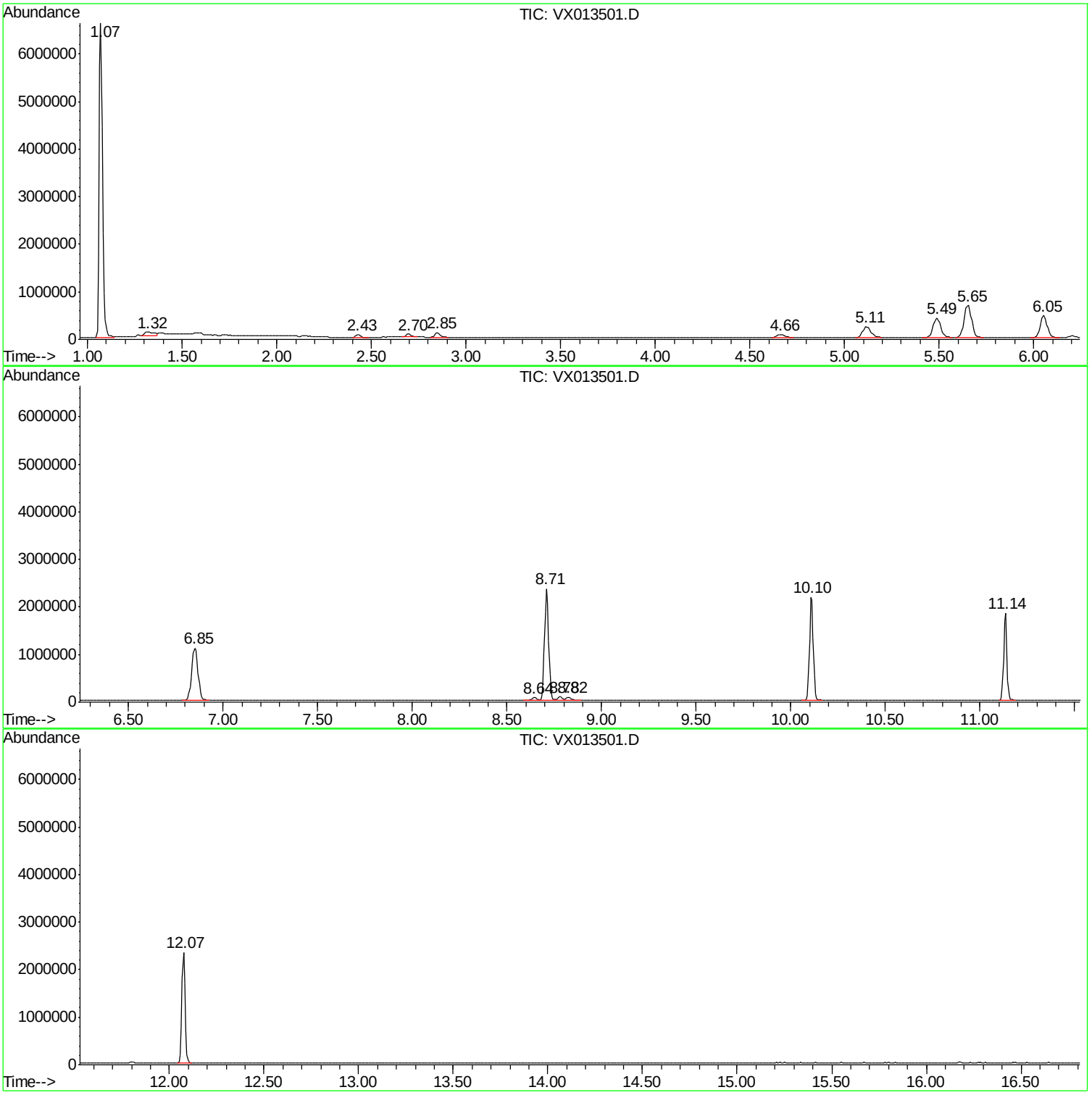
Instrument : MSVOA_X
ClientSampleId : FERMENTATION-WASTE

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X103119W.M
Quant Title : SW846 8260

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX112119\
Data File : VX013501.D
Acq On : 21 Nov 2019 14:27
Operator : JC/SP
Sample : K5967-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FERMENTATION-WASTE

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X103119W.M
Quant Title : SW846 8260

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

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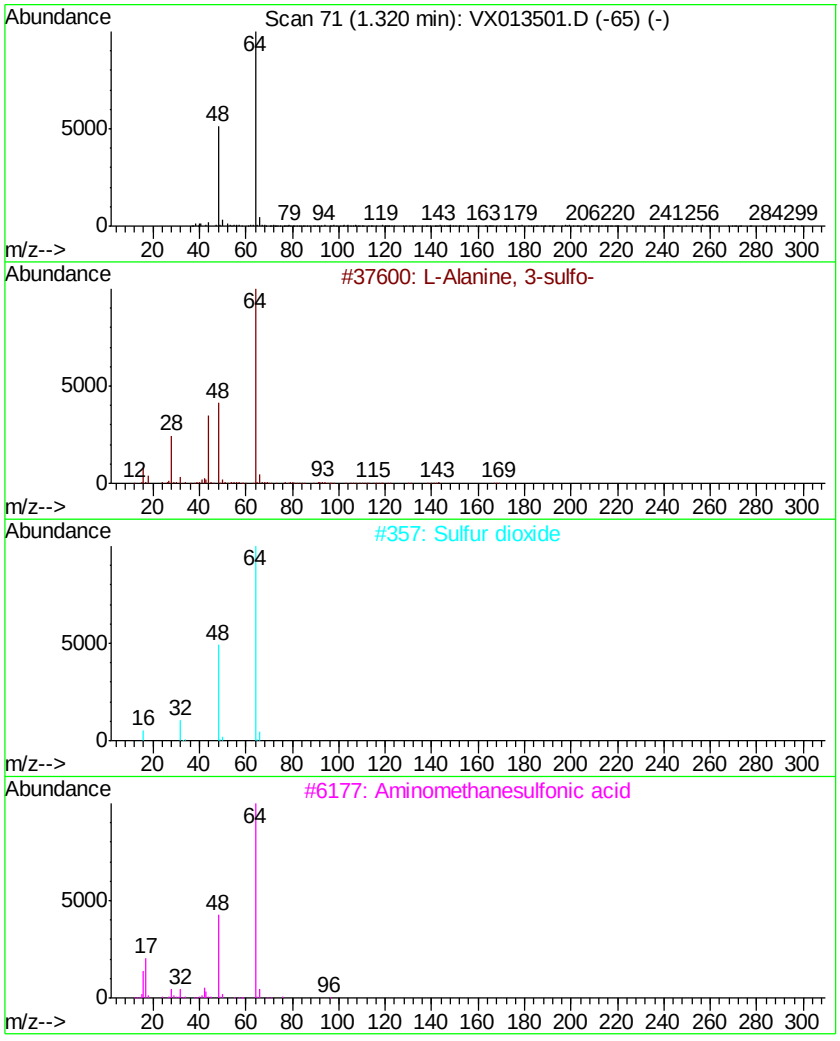
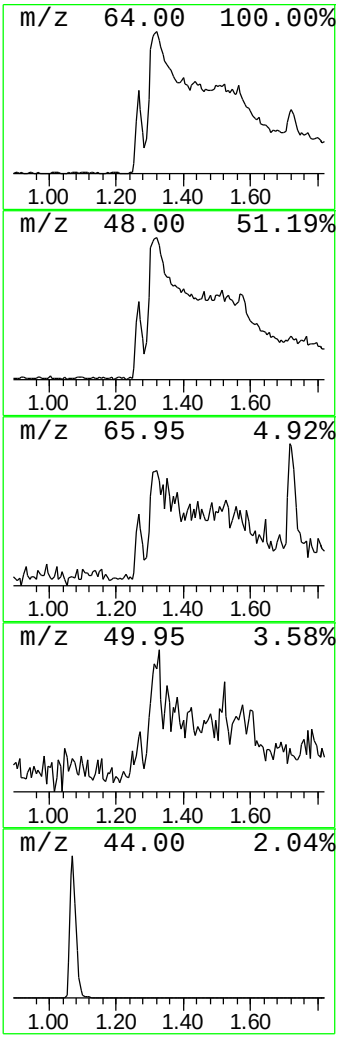
Peak Number 2 L-Alanine, 3-sulfo- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.32	8.71 ug/l	328917	Pentafluorobenzene	5.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	90
2	Sulfur dioxide	64	O2S	007446-09-5	90
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
4	2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74
5	Dibenzo[cd,g]indazole-3-sulfonic...	300	C14H8N2O4S	293765-87-4	64





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
L-Alanine, 3-sulfo-	1.32	8.7	ug/l	328917	1	5.65	1888400	50.0