

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX122719\
 Data File : VX014313.D
 Acq On : 27 Dec 2019 16:54
 Operator : JC/SP
 Sample : K6434-06
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 GW-5

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.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	44	rBV	3238346	3756209	100.00%	22.819%
2	1.265	59	62	67	rBV	29037	39263	1.05%	0.239%
3	1.326	67	72	80	rBV3	61537	232097	6.18%	1.410%
4	2.588	273	279	285	rBV	23716	45721	1.22%	0.278%
5	5.490	743	755	767	rBV	270728	769689	20.49%	4.676%
6	5.655	772	782	795	rBV	490165	1359562	36.20%	8.259%
7	6.057	837	848	859	rBV	319152	809194	21.54%	4.916%
8	6.849	968	978	991	rBV	755894	1755129	46.73%	10.662%
9	8.709	1276	1283	1292	rBV	1580327	2416148	64.32%	14.678%
10	10.111	1507	1513	1522	rBV	1453686	2024939	53.91%	12.302%
11	11.135	1675	1681	1691	rBV	1142456	1491892	39.72%	9.063%
12	12.074	1828	1835	1845	rBV	1417693	1761002	46.88%	10.698%

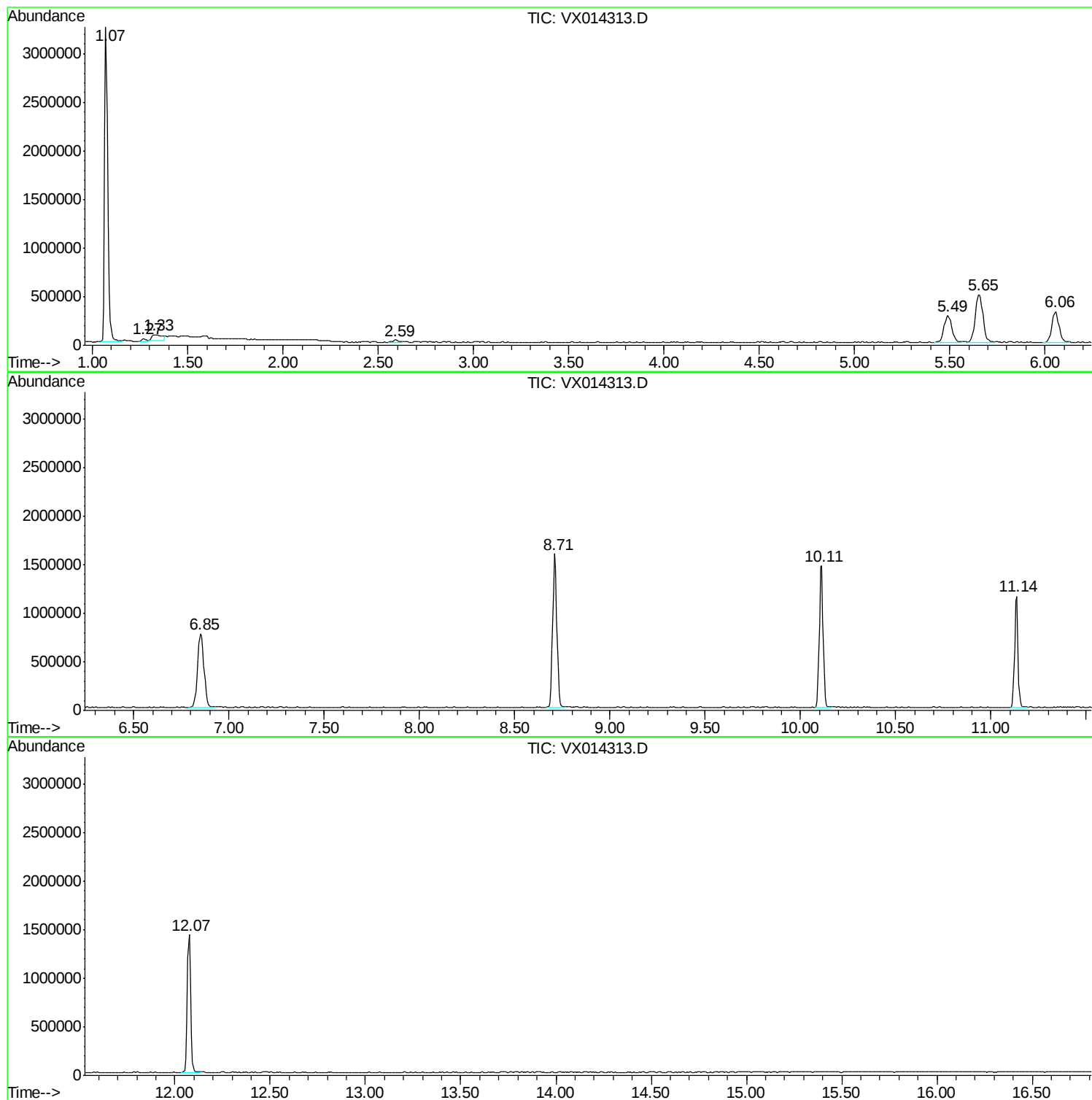
Sum of corrected areas: 16460845

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121319W.M
Quant Title : SW846 8260

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



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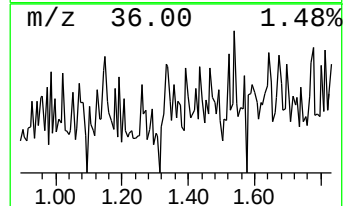
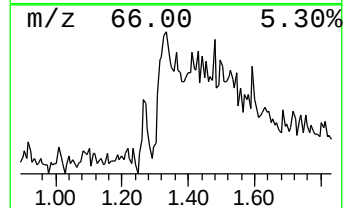
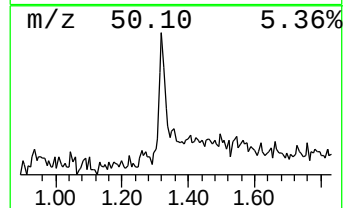
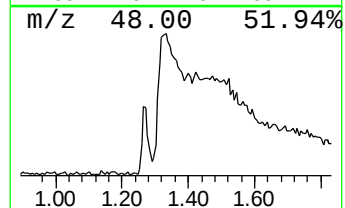
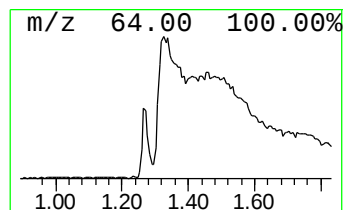
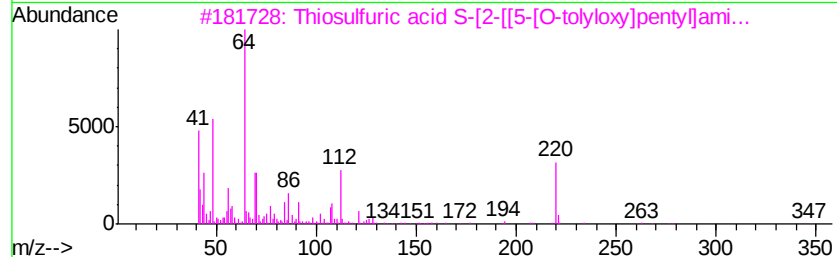
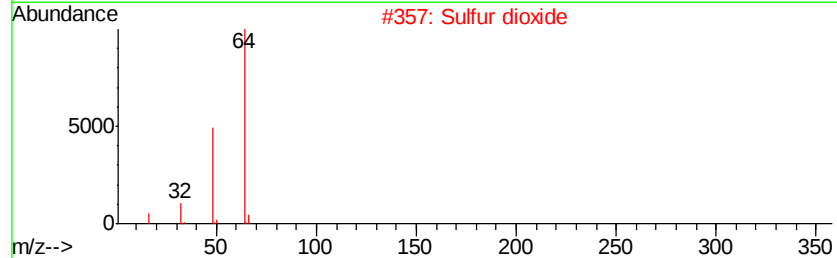
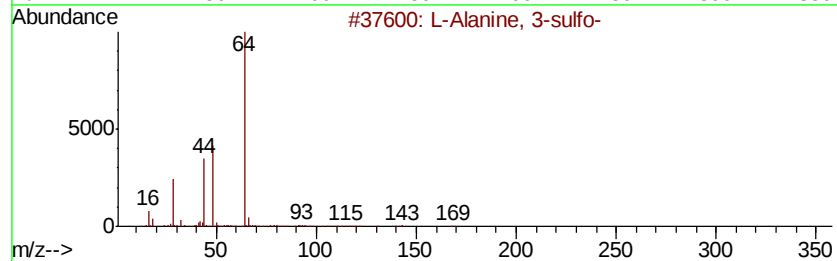
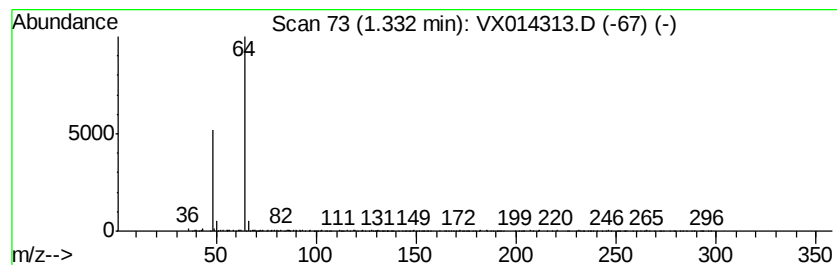
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.33	8.54 ug/l	232097	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	83
2		Sulfur dioxide	64	O2S	007446-09-5	74
3		Thiosulfuric acid S-[2-[5-[O-to...	347	C15H25N04S2	038920-47-7	64
4		Dibenzo[cd,qlindazole-3-sulfonic...	300	C14H8N2O4S	293765-87-4	64
5		Thiosulfuric acid (H2S2O3), S-(2...	320	C11H16N2O3S3	040284-00-2	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
L-Alanine, 3-sulfo-	1.33	8.5	ug/l	232097	1	5.65	1359560	50.0