

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041222\
 Data File : VX028074.D
 Acq On : 12 Apr 2022 22:13
 Operator : JC/MD
 Sample : N2334-09
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-21RR

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\82X041222W.M
 Title : SW846 8260

Signal : TIC: VX028074.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	24	29	44	rBV	39089	166417	14.24%	2.400%
2	1.557	70	77	83	rVB2	47619	106176	9.08%	1.531%
3	1.752	105	109	114	rVB4	6704	11839	1.01%	0.171%
4	2.532	231	237	243	rBV2	12293	24252	2.07%	0.350%
5	2.782	272	278	284	rBV4	9397	20225	1.73%	0.292%
6	5.385	694	705	719	rBV	136832	405363	34.68%	5.846%
7	5.556	723	733	754	rVB	212976	636794	54.47%	9.183%
8	5.958	788	799	812	rBV	145433	397897	34.04%	5.738%
9	6.245	838	846	857	rVB3	14327	46555	3.98%	0.671%
10	6.763	921	931	942	rBV	351390	824437	70.52%	11.889%
11	7.367	1020	1030	1038	rBV6	5472	14838	1.27%	0.214%
12	7.982	1123	1131	1138	rVB	16979	32544	2.78%	0.469%
13	8.110	1141	1152	1162	rBV2	26234	60606	5.18%	0.874%
14	8.653	1226	1241	1254	rBV	738470	1169016	100.00%	16.859%
15	10.055	1465	1471	1480	rBV	779434	1034576	88.50%	14.920%
16	10.963	1615	1620	1626	rBV	12919	17891	1.53%	0.258%
17	11.079	1634	1639	1650	rBV	589007	781982	66.89%	11.277%
18	11.305	1671	1676	1682	rVB	12653	17720	1.52%	0.256%
19	12.024	1788	1794	1803	rBV	810425	984039	84.18%	14.191%
20	12.244	1823	1830	1836	rVB	34093	45711	3.91%	0.659%
21	12.701	1901	1905	1912	rVB6	10441	16813	1.44%	0.242%
22	12.920	1933	1941	1946	rBV	31020	44116	3.77%	0.636%
23	13.134	1973	1976	1980	rBV2	11780	16273	1.39%	0.235%
24	13.853	2090	2094	2098	rVB3	11320	14640	1.25%	0.211%
25	13.926	2098	2106	2111	rBV3	9284	15456	1.32%	0.223%
26	14.323	2166	2171	2176	rBV3	9807	14562	1.25%	0.210%
27	14.786	2242	2247	2251	rBV3	9279	13477	1.15%	0.194%

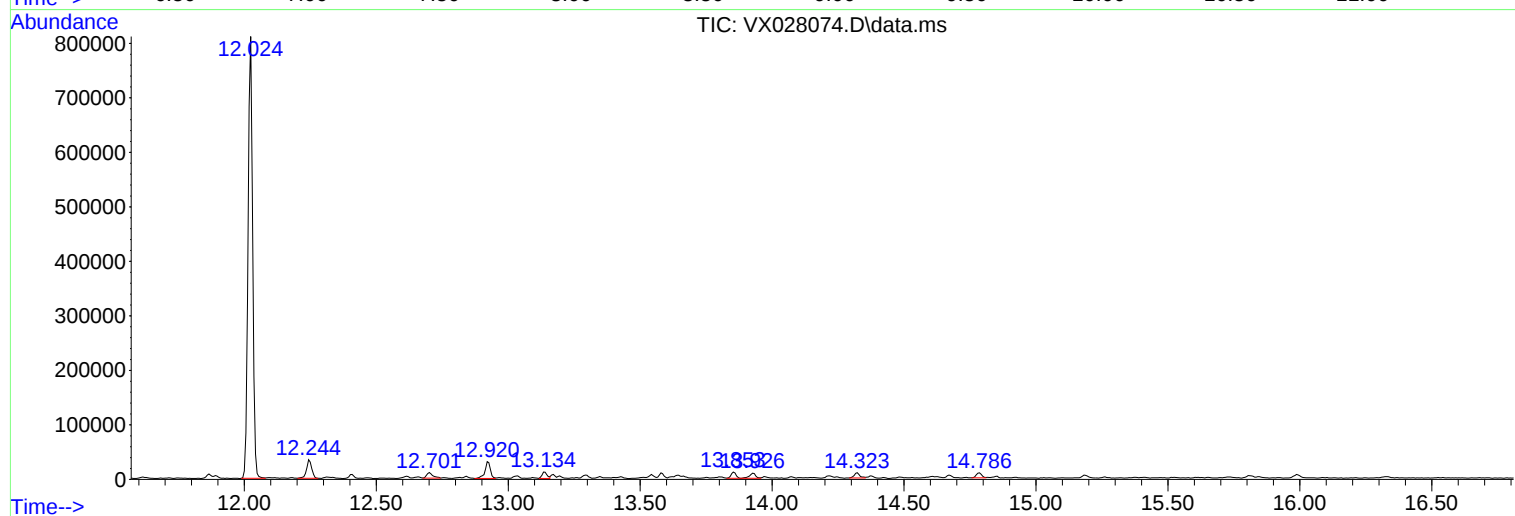
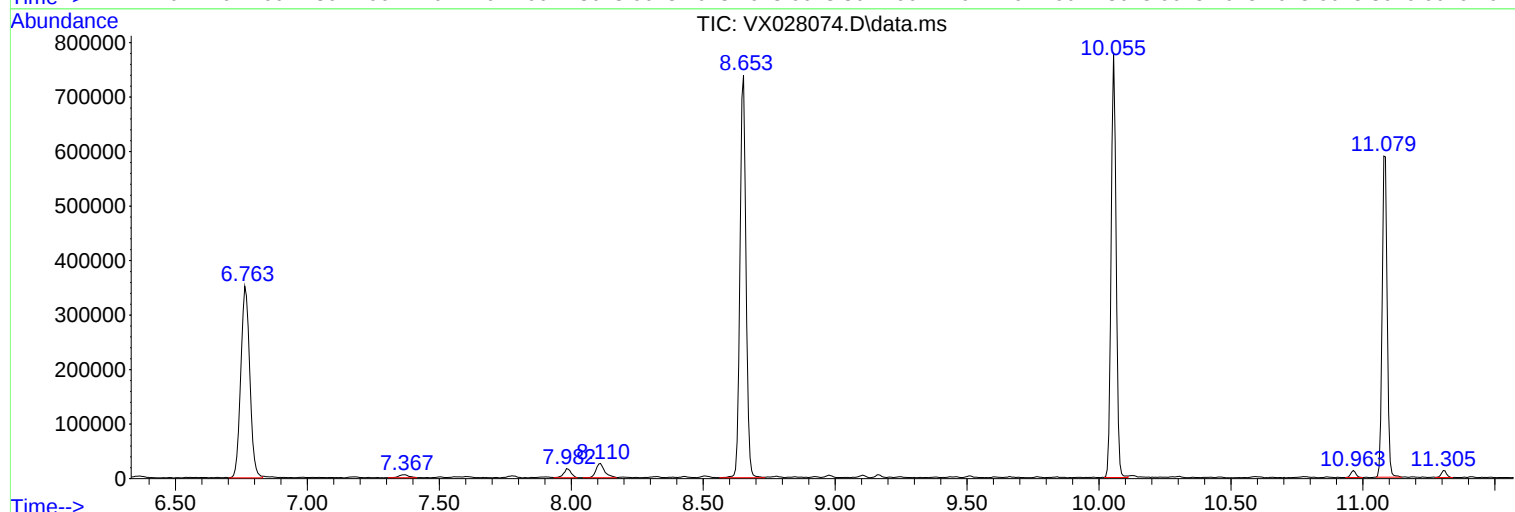
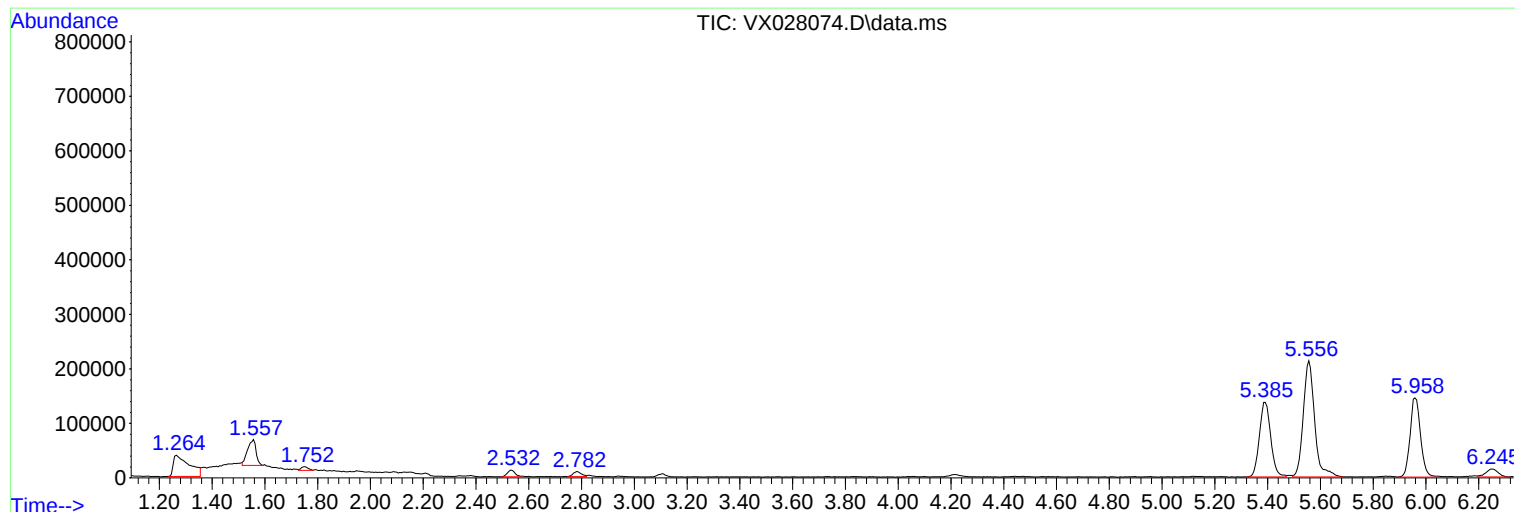
Sum of corrected areas: 6934215

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Instrument :
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ClientSampleId :
MW-21RR

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041222W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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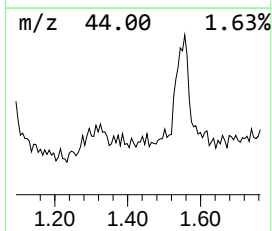
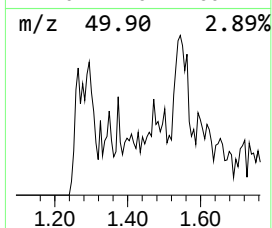
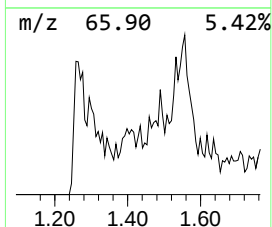
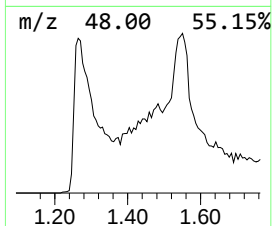
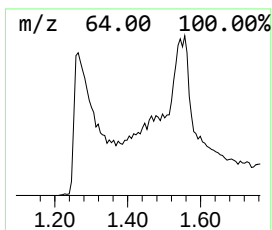
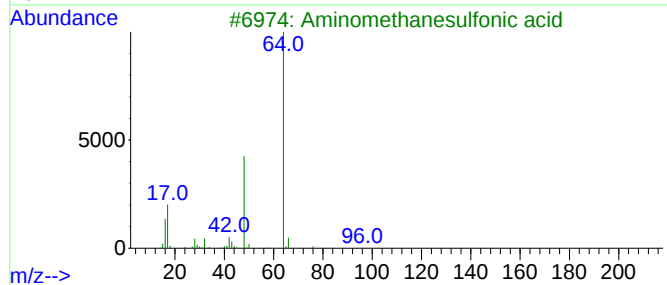
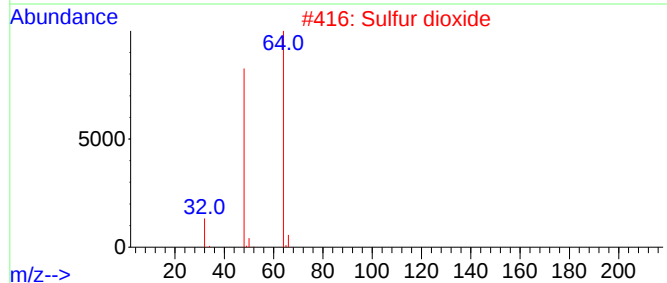
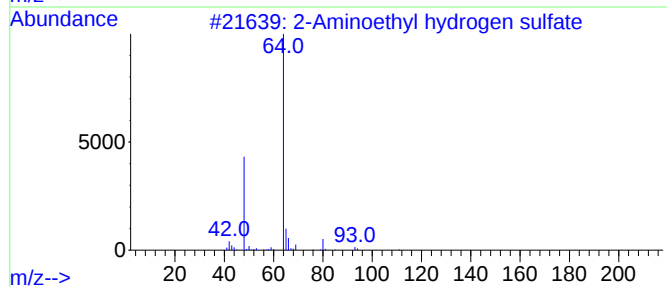
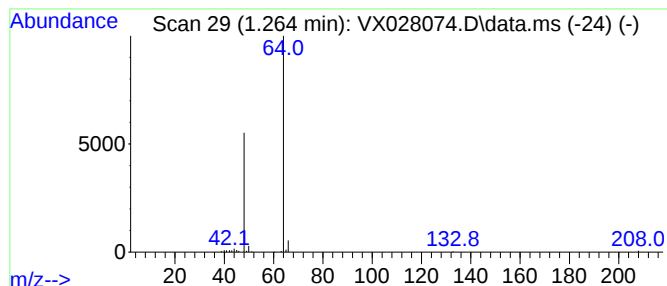
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X041222W.M
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TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Aminoethyl hydrogen sulfate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	13.07 ug/l	166417	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	83
2			Sulfur dioxide	64	O2S	007446-09-5	83
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
4			1,1,1,2,2,3,3,4,4,5,5-Undecafluorooctane	602	C10F22O2S	1000486-78-5	74
5			2-Benzimidazolyl methane thiosulfonate	244	C8H8N2O3S2	1010256-39-2	9



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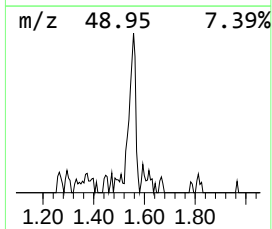
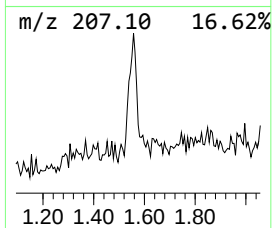
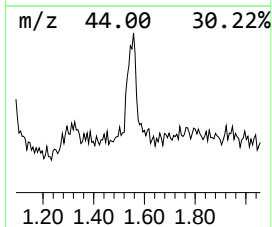
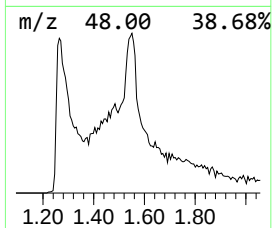
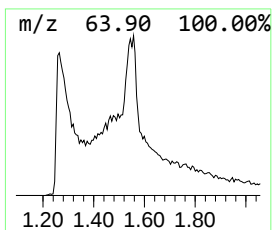
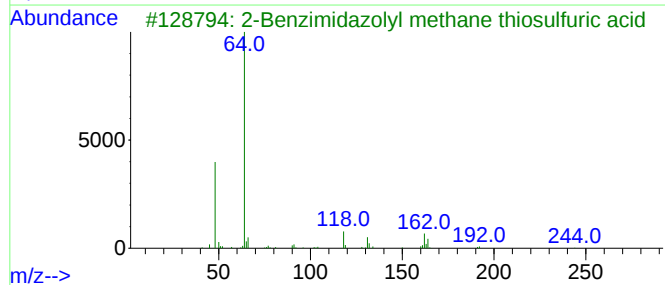
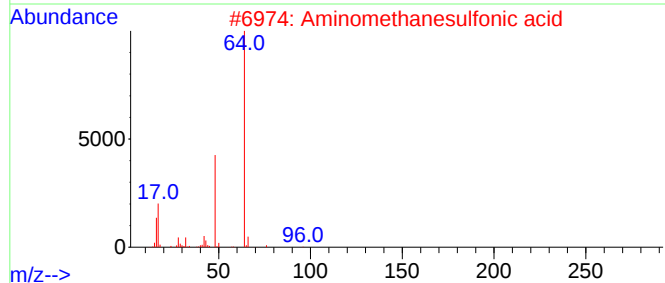
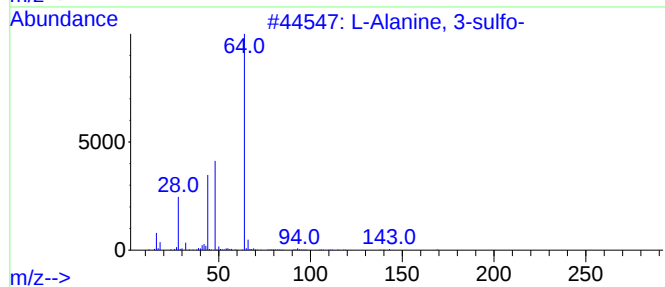
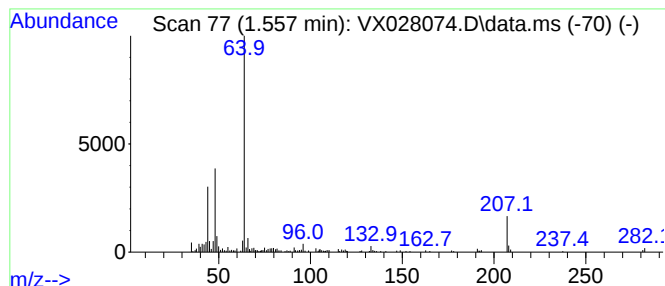
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Peak Number 2 L-Alanine, 3-sulfo- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.557	8.34 ug/l	106176	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	78
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	72
3			2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1010256-39-2	72
4			4,6-Diamino-5-pyrimidinyl hydrog...	206	C4H6N4O4S	071525-41-2	64
5			2,4,6-Triamino-5-pyrimidinyl hyd...	221	C4H7N5O4S	071552-23-3	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Aminoethyl hy...	1.264	13.1	ug/l	166417	1	5.556	636794	50.0
L-Alanine, 3-su...	1.557	8.3	ug/l	106176	1	5.556	636794	50.0