

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082923\
 Data File : VX037345.D
 Acq On : 29 Aug 2023 16:28
 Operator : JC/MD
 Sample : 04208-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BR-03-127-082823-H

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\82X081723W.M
 Title : SW846 8260

Signal : TIC: VX037345.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	22	28	41	rBV	23210	74755	10.78%	1.523%
2	2.130	169	171	179	rVB5	3239	6970	1.01%	0.142%
3	2.313	195	201	208	rBV	87246	135705	19.57%	2.765%
4	2.386	208	213	221	rVB	9316	16731	2.41%	0.341%
5	2.550	229	240	253	rBV	20481	42009	6.06%	0.856%
6	3.093	323	329	338	rBV	5616	11154	1.61%	0.227%
7	3.611	402	414	425	rVB	7270	18369	2.65%	0.374%
8	4.489	547	558	571	rBV2	58526	160817	23.19%	3.277%
9	5.385	692	705	721	rBV	80420	232551	33.53%	4.739%
10	5.550	721	732	748	rVV	149522	421327	60.75%	8.586%
11	5.958	788	799	814	rBV2	84604	231525	33.38%	4.718%
12	6.092	814	821	834	rVB2	4843	14541	2.10%	0.296%
13	6.763	921	931	947	rBV	217212	518392	74.75%	10.564%
14	7.123	982	990	1005	rBV	285263	620117	89.42%	12.637%
15	8.647	1234	1240	1250	rBV	441979	693525	100.00%	14.133%
16	10.055	1465	1471	1488	rBV	439734	593628	85.60%	12.097%
17	11.079	1634	1639	1652	rBV	355314	450680	64.98%	9.184%
18	12.024	1788	1794	1808	rBV	426297	555419	80.09%	11.318%
19	12.219	1821	1826	1841	rBV	60418	109043	15.72%	2.222%

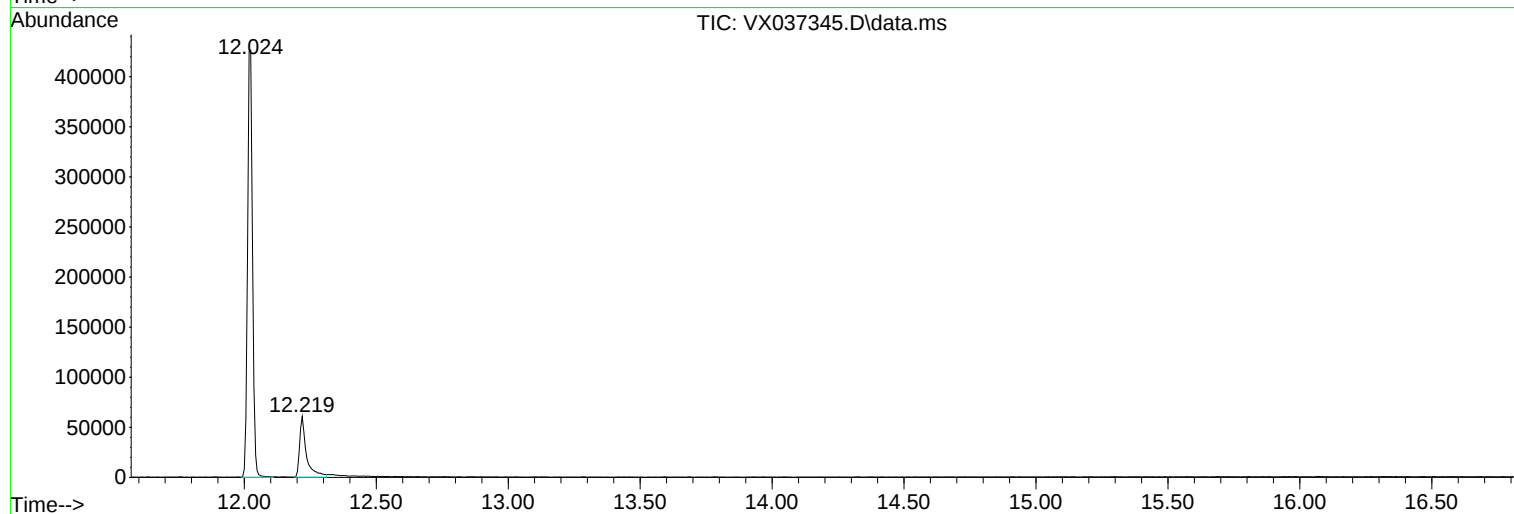
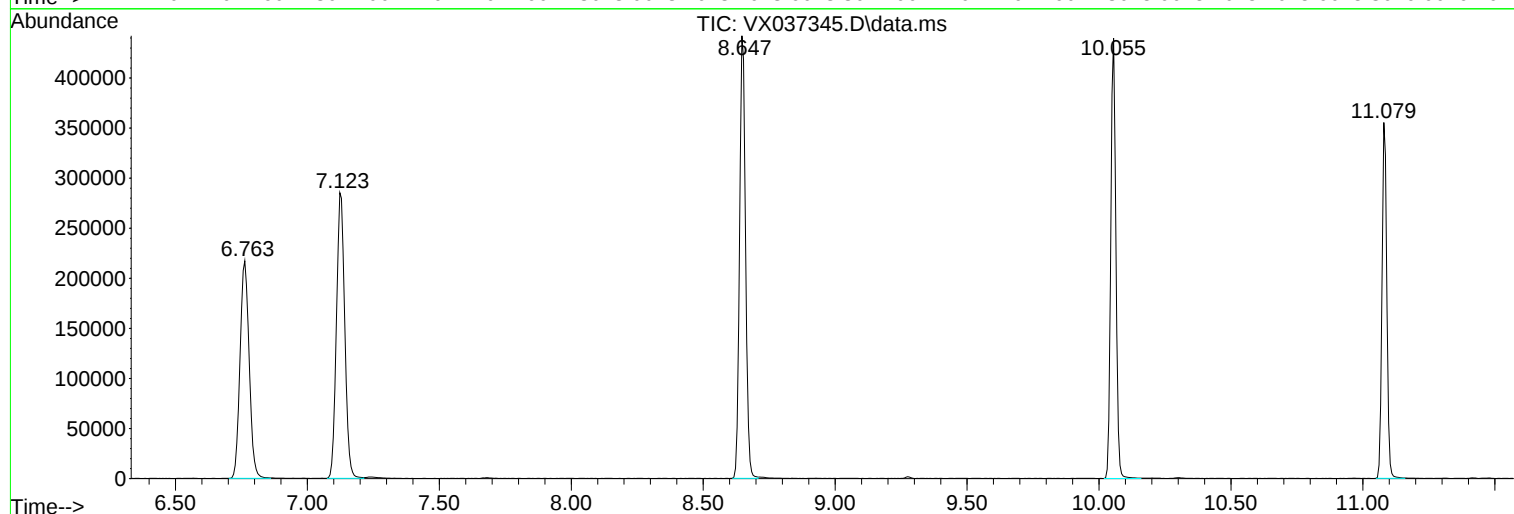
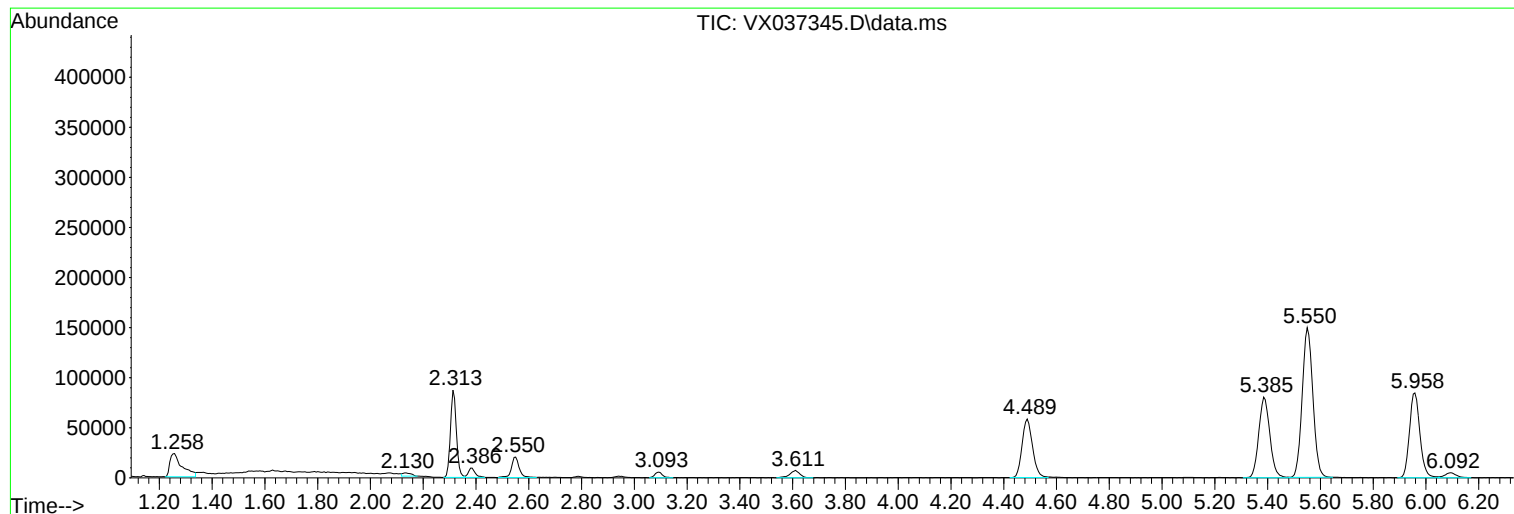
Sum of corrected areas: 4907258

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Quant Title : SW846 8260

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



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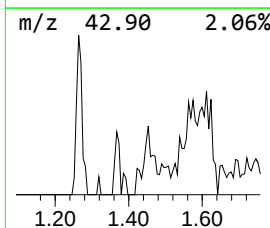
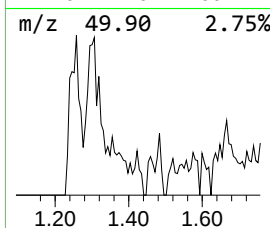
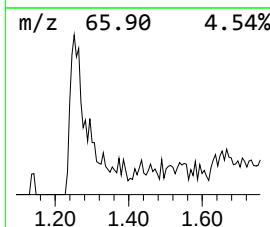
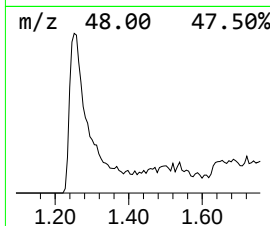
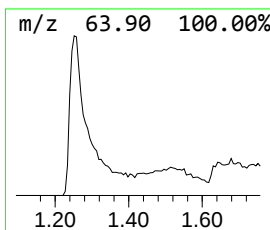
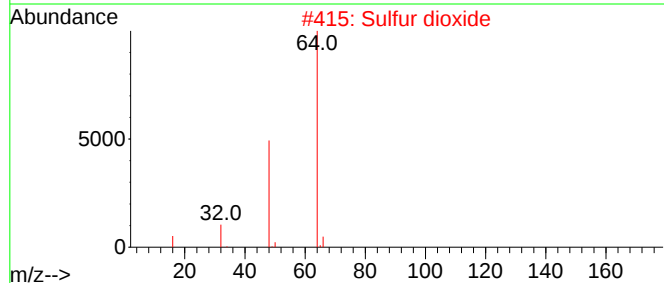
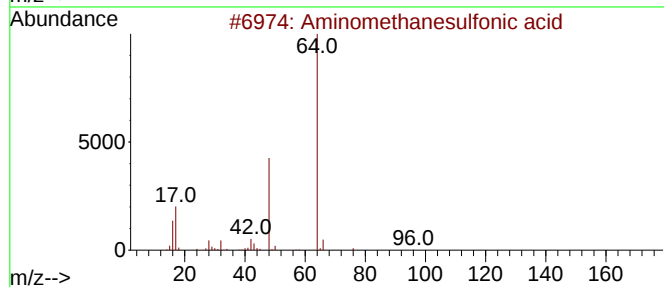
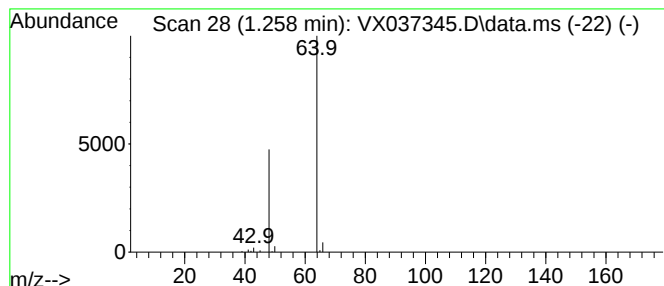
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Peak Number 1 Aminomethanesulfonic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	8.87 ug/l	74755	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	83
2			Sulfur dioxide	64	O2S	007446-09-5	83
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5
5			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	4



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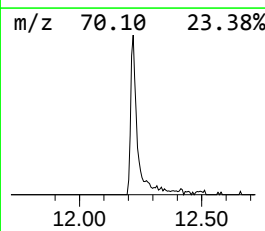
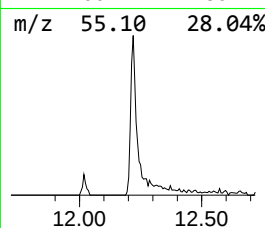
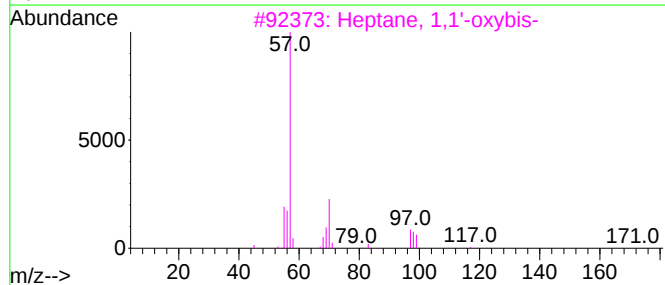
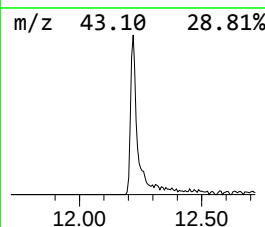
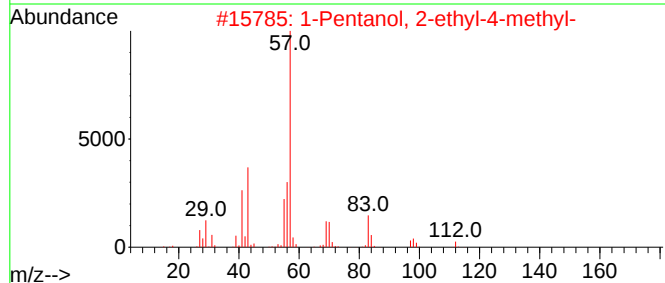
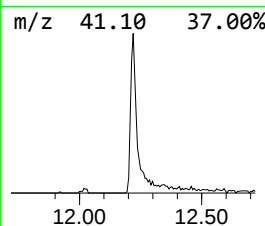
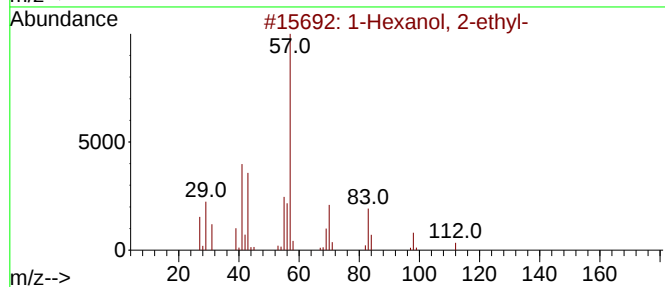
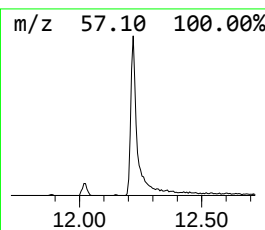
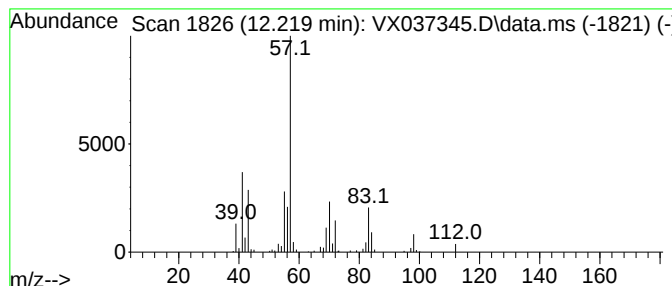
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Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	9.82 ug/l	109043	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	86
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	47
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
5			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	40



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Aminomethanesul...	1.258	8.9	ug/l	74755	1	5.550	421327	50.0
1-Hexanol, 2-et...	12.219	9.8	ug/l	109043	4	12.024	555419	50.0