

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
 Data File : VN074538.D
 Acq On : 17 Sep 2022 03:20
 Operator : JC\MD
 Sample : N4549-10
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-54

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_N\methods\82N091522W.M
 Title : SW846 8260

Signal : TIC: VN074538.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	47	53	61	rBV	252925	500304	25.58%	4.151%
2	2.687	131	136	141	rBV	65335	175582	8.98%	1.457%
3	2.734	142	144	152	rVB2	78364	97689	4.99%	0.811%
4	5.275	563	576	596	rVB3	75816	276665	14.14%	2.296%
5	5.528	604	619	631	rBV4	66820	250148	12.79%	2.076%
6	6.410	760	769	777	rBV2	19439	53539	2.74%	0.444%
7	7.951	1021	1031	1036	rBV	265230	638079	32.62%	5.295%
8	8.016	1036	1042	1053	rVB	416939	930628	47.58%	7.722%
9	8.369	1092	1102	1112	rBV2	309521	701693	35.87%	5.822%
10	8.469	1112	1119	1127	rVB6	15773	40903	2.09%	0.339%
11	8.904	1182	1193	1203	rBV	687414	1401295	71.64%	11.628%
12	10.380	1437	1444	1457	rBV	1102973	1955956	100.00%	16.230%
13	11.686	1657	1666	1677	rBV	1107522	1897570	97.01%	15.745%
14	12.674	1826	1834	1842	rBV	875947	1432524	73.24%	11.887%
15	13.615	1986	1994	2004	rBV	1032062	1698948	86.86%	14.097%

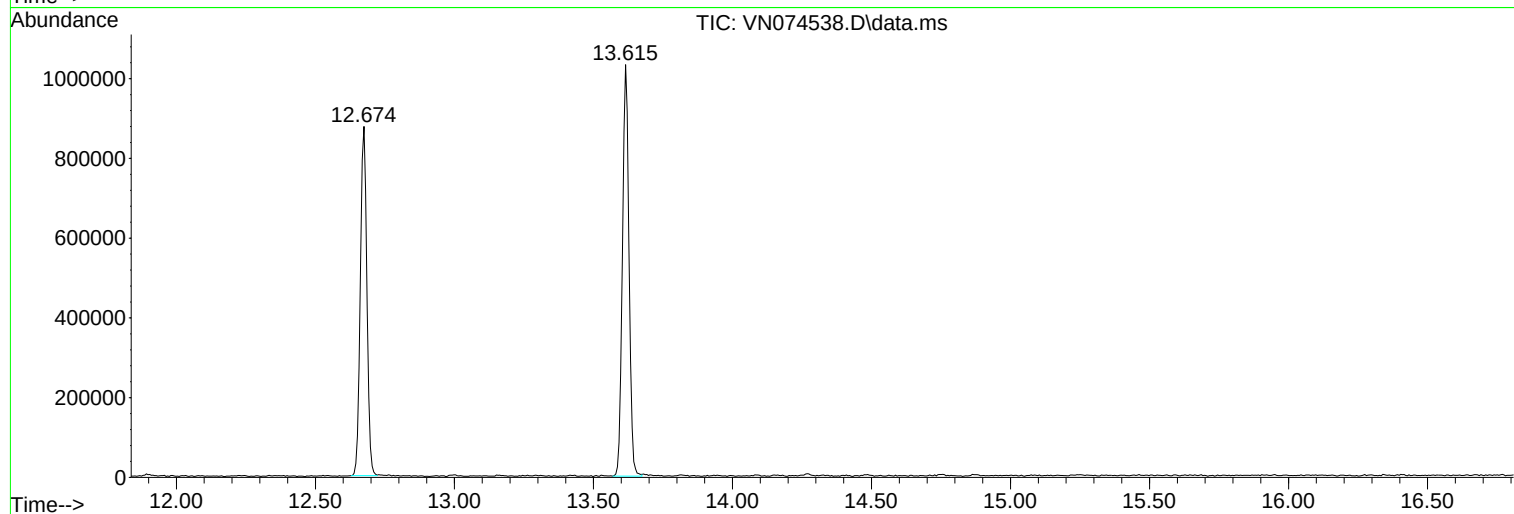
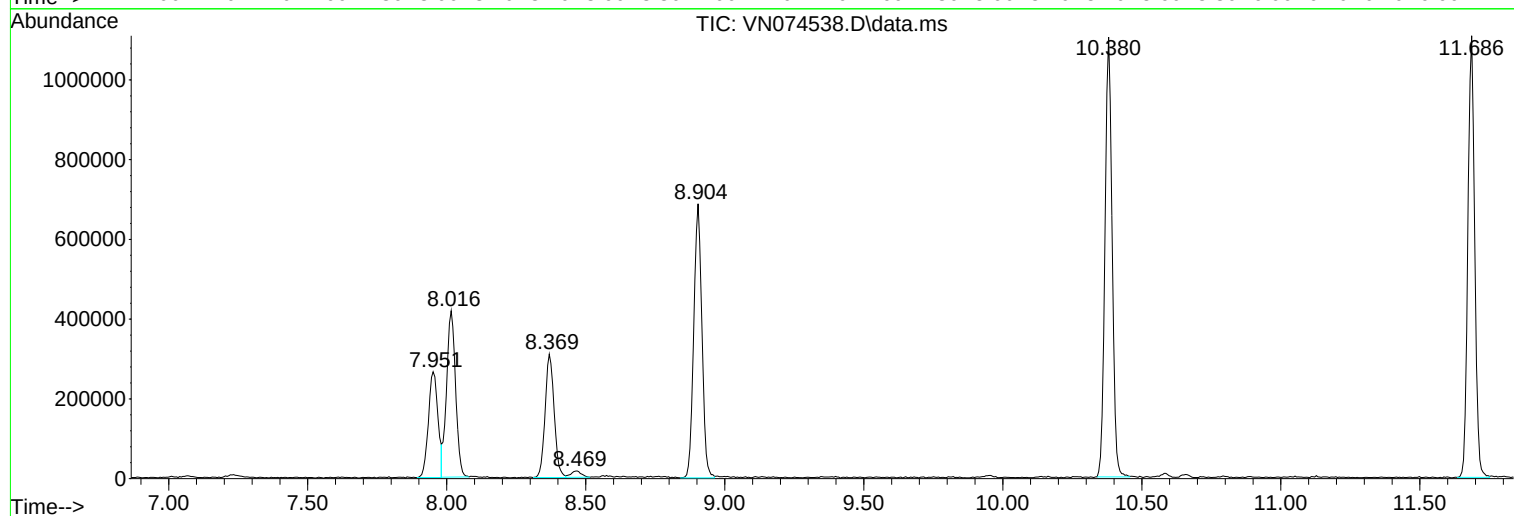
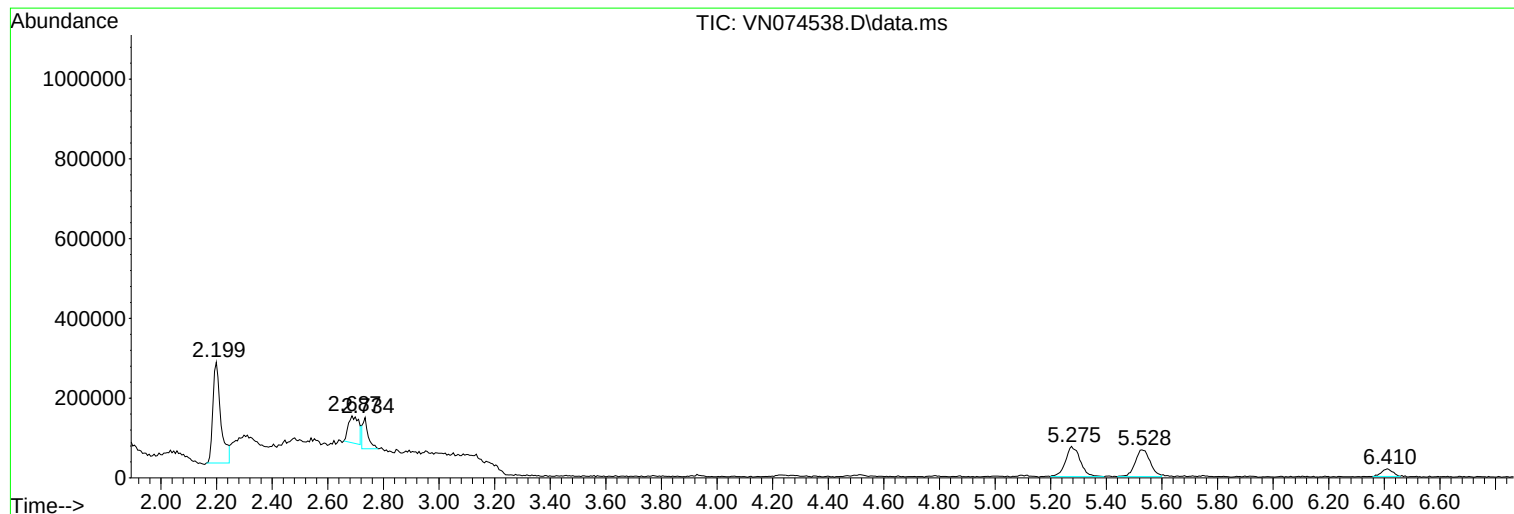
Sum of corrected areas: 12051523

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074538.D
Acq On : 17 Sep 2022 03:20
Operator : JC\MD
Sample : N4549-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-54

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074538.D
Acq On : 17 Sep 2022 03:20
Operator : JC\MD
Sample : N4549-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-54

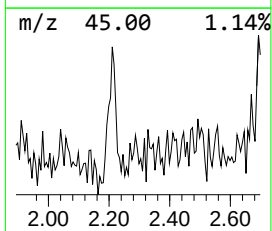
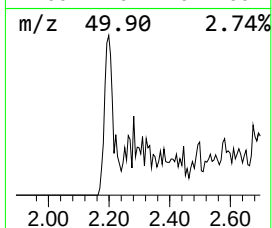
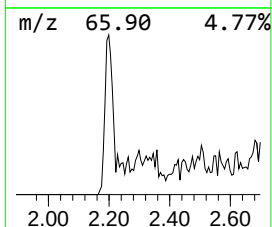
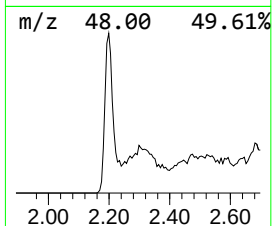
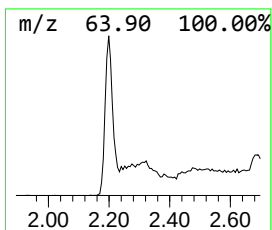
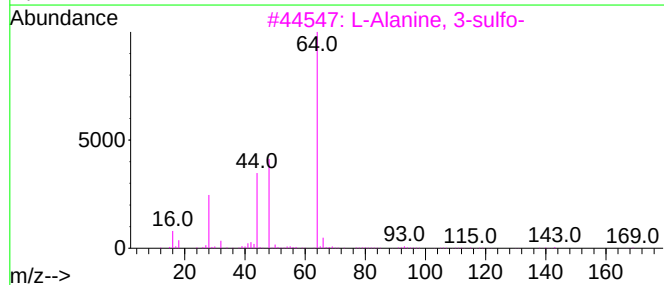
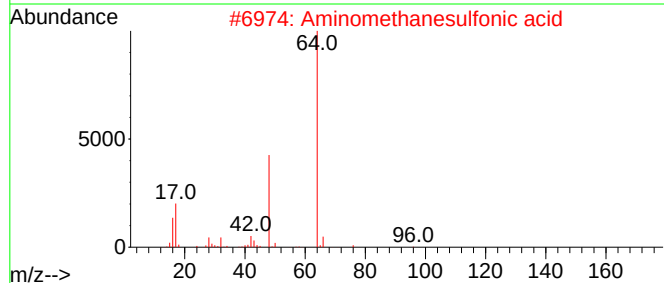
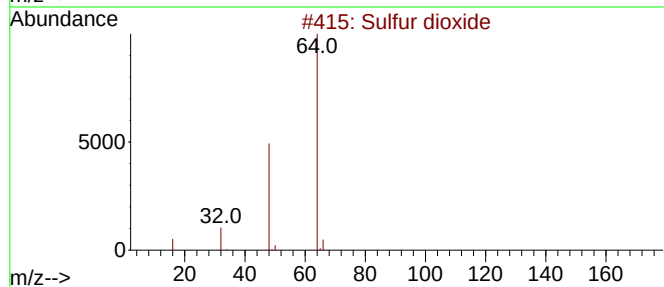
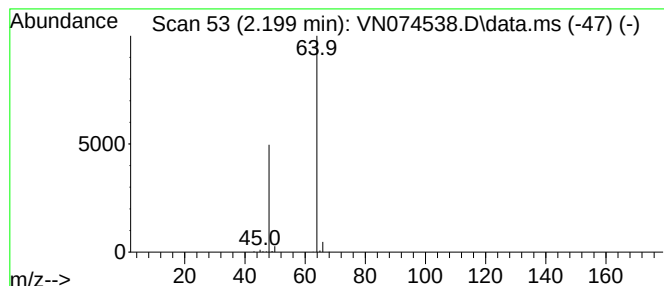
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	26.88 ug/l	500304	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074538.D
Acq On : 17 Sep 2022 03:20
Operator : JC\MD
Sample : N4549-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-54

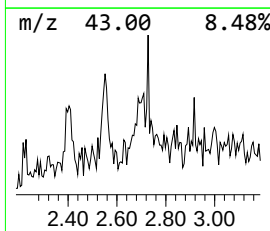
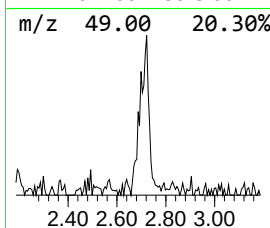
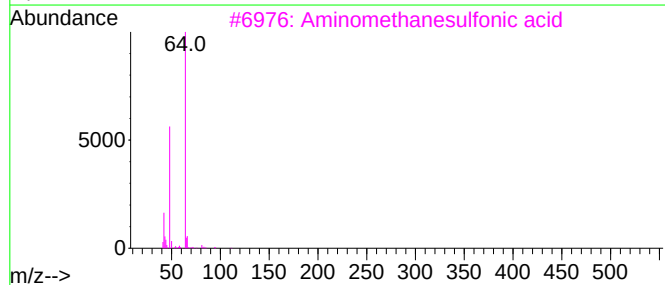
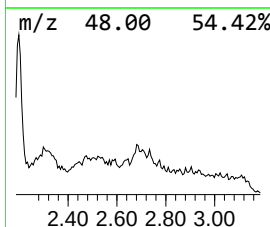
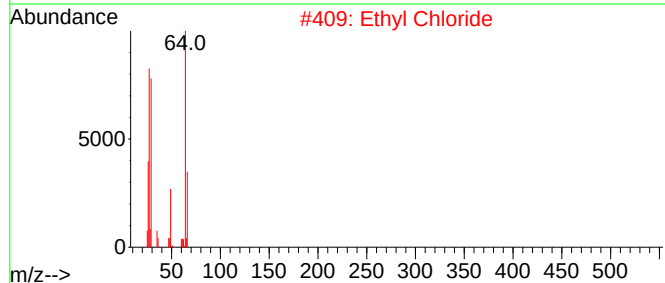
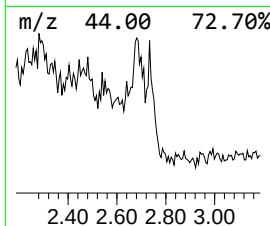
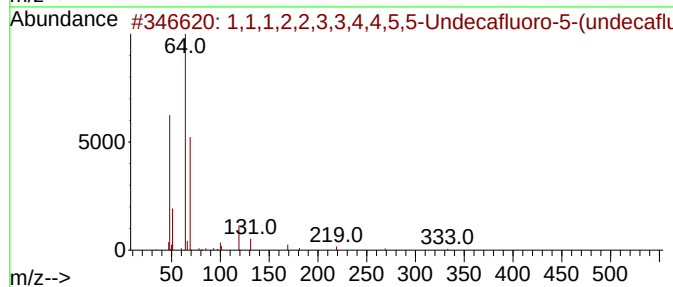
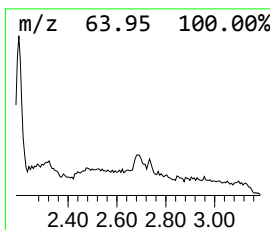
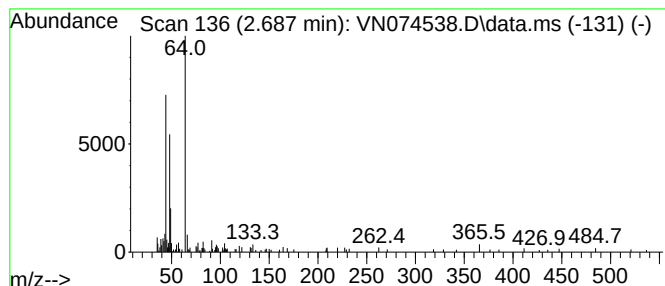
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethyl Chloride Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.687	9.43 ug/l	175582	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,1,2,2,3,3,4,4,5,5-Undecafluoro-5-(undecafluoroethyl)benzene	602	C10F22O2S	1000486-78-5	64		
2	Ethyl Chloride	64	C2H5Cl	000075-00-3	64		
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	59		
4	Dibenzo[cd,g]indazole-3-sulfonic acid	300	C14H8N2O4S	293765-87-4	53		
5	Sulfur dioxide	64	O2S	007446-09-5	42		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074538.D
Acq On : 17 Sep 2022 03:20
Operator : JC\MD
Sample : N4549-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-54

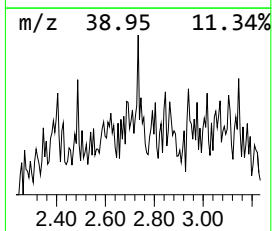
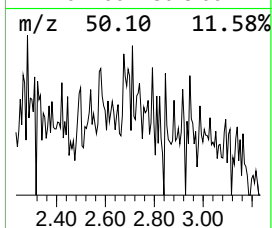
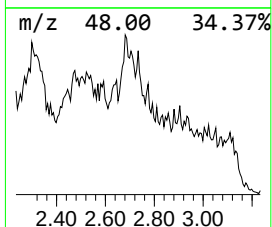
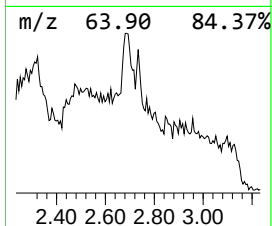
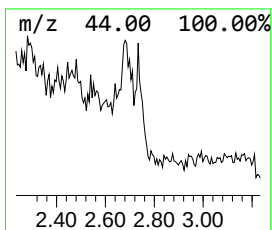
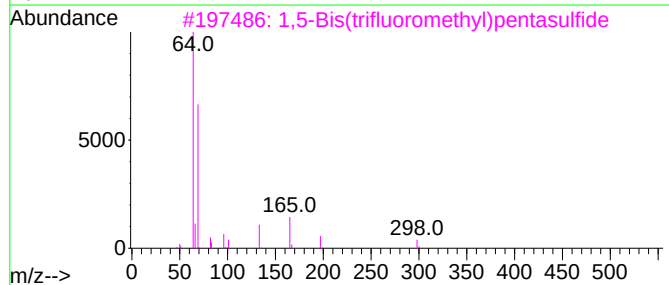
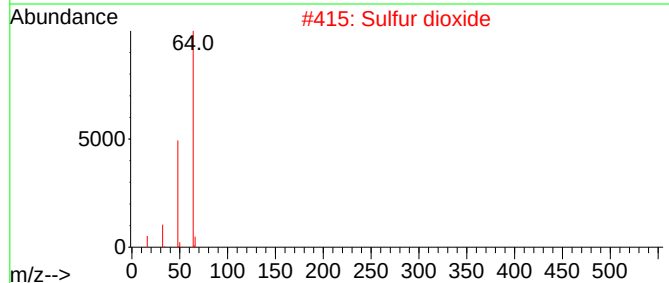
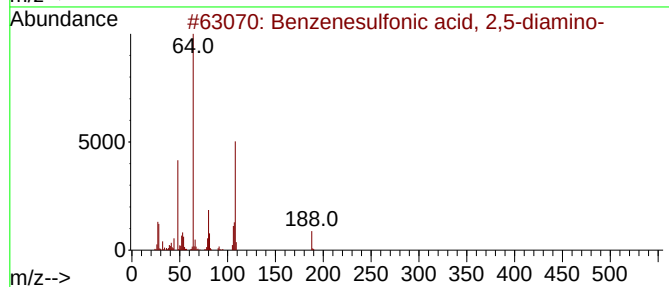
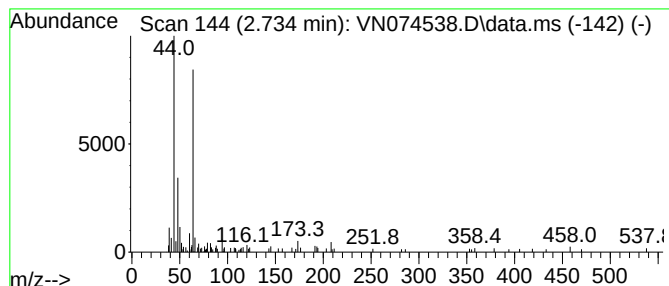
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

Peak Number 3 unknown2.734 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.734	5.25 ug/l	97689	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonic acid, 2,5-diamino-	188	C6H8N2O3S	000088-45-9	45
2			Sulfur dioxide	64	O2S	007446-09-5	45
3			1,5-Bis(trifluoromethyl)pentasul...	298	C2F6S5	156412-87-2	43
4			4,4'-Diaminostilbene-2,2'-disulf...	370	C14H14N2O6S2	000081-11-8	39
5			Thiosulfuric acid S-[2-[[5-[O-to...	347	C15H25N04S2	038920-47-7	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
Data File : VN074538.D
Acq On : 17 Sep 2022 03:20
Operator : JC\MD
Sample : N4549-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 44 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-54

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.199	26.9	ug/l	500304	1	8.016	930628	50.0
Ethyl Chloride	2.687	9.4	ug/l	175582	1	8.016	930628	50.0
unknown2.734	2.734	5.3	ug/l	97689	1	8.016	930628	50.0