

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU103122\
 Data File : VU051640.D
 Acq On : 01 Nov 2022 03:41
 Operator : JC/MD
 Sample : N5319-17
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHAB2

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.1

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_U\Method\SFAMUTR102822WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU051640.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.465	30	39	52	rBV	252959	446394	41.69%	6.019%
2	1.597	75	80	125	rVB2	130044	352602	32.93%	4.755%
3	1.909	170	177	192	rVB	89273	120588	11.26%	1.626%
4	2.565	369	381	393	rBV	114756	187262	17.49%	2.525%
5	2.755	430	440	451	rBV2	9022	18069	1.69%	0.244%
6	3.044	517	530	541	rBV4	5960	12311	1.15%	0.166%
7	3.179	560	572	587	rVB2	12332	27343	2.55%	0.369%
8	3.362	616	629	643	rBV3	11693	25772	2.41%	0.348%
9	3.906	765	798	818	rVB	12048	59015	5.51%	0.796%
10	4.620	1005	1020	1060	rBV2	187674	487067	45.49%	6.568%
11	5.063	1141	1158	1179	rBV	174436	417927	39.03%	5.635%
12	5.722	1341	1363	1393	rBV2	300716	825479	77.09%	11.131%
13	6.247	1512	1526	1550	rBV	214632	416341	38.88%	5.614%
14	6.690	1649	1664	1687	rBV	218153	427091	39.88%	5.759%
15	7.163	1799	1811	1833	rBV9	5951	15104	1.41%	0.204%
16	7.565	1921	1936	1951	rBV2	59884	104870	9.79%	1.414%
17	7.896	2024	2039	2056	rBV	269701	475122	44.37%	6.407%
18	8.179	2117	2127	2148	rBV	38298	66529	6.21%	0.897%
19	8.632	2255	2268	2299	rBV2	566761	1070809	100.00%	14.439%
20	9.417	2499	2512	2536	rBV	332585	564316	52.70%	7.609%
21	10.754	2916	2928	2945	rBV	199234	319680	29.85%	4.311%
22	11.809	3245	3256	3277	rBV	265569	433120	40.45%	5.840%
23	12.192	3362	3375	3394	rBV	263182	439458	41.04%	5.926%
24	16.764	4785	4797	4818	rBV2	62667	103769	9.69%	1.399%

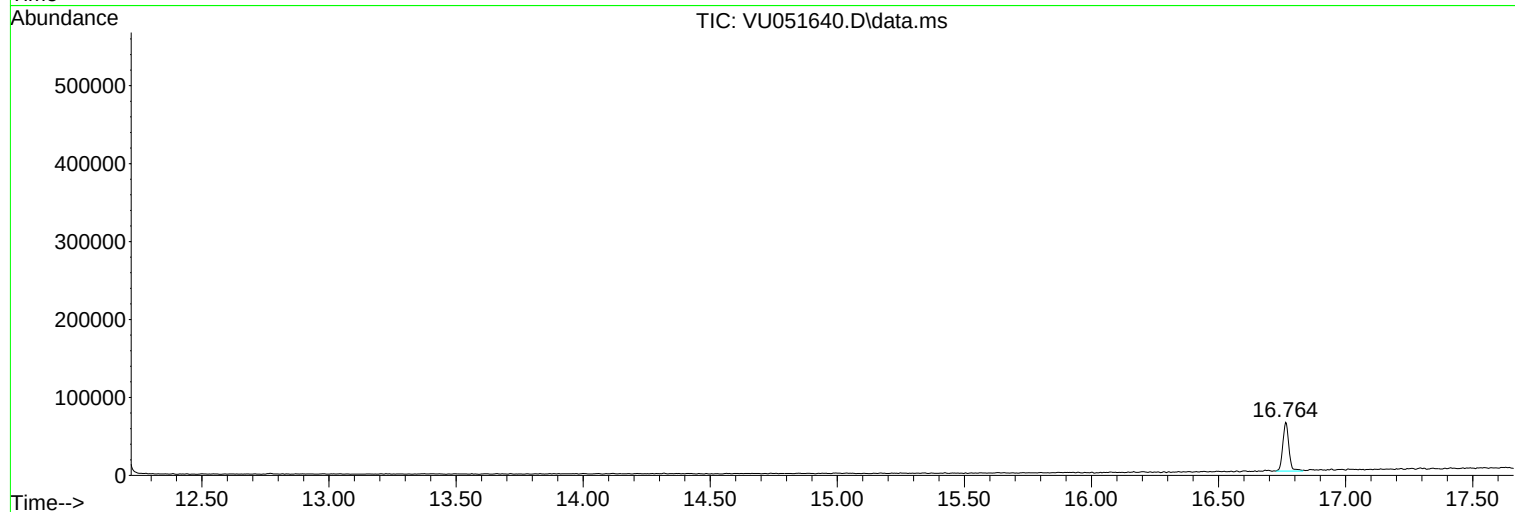
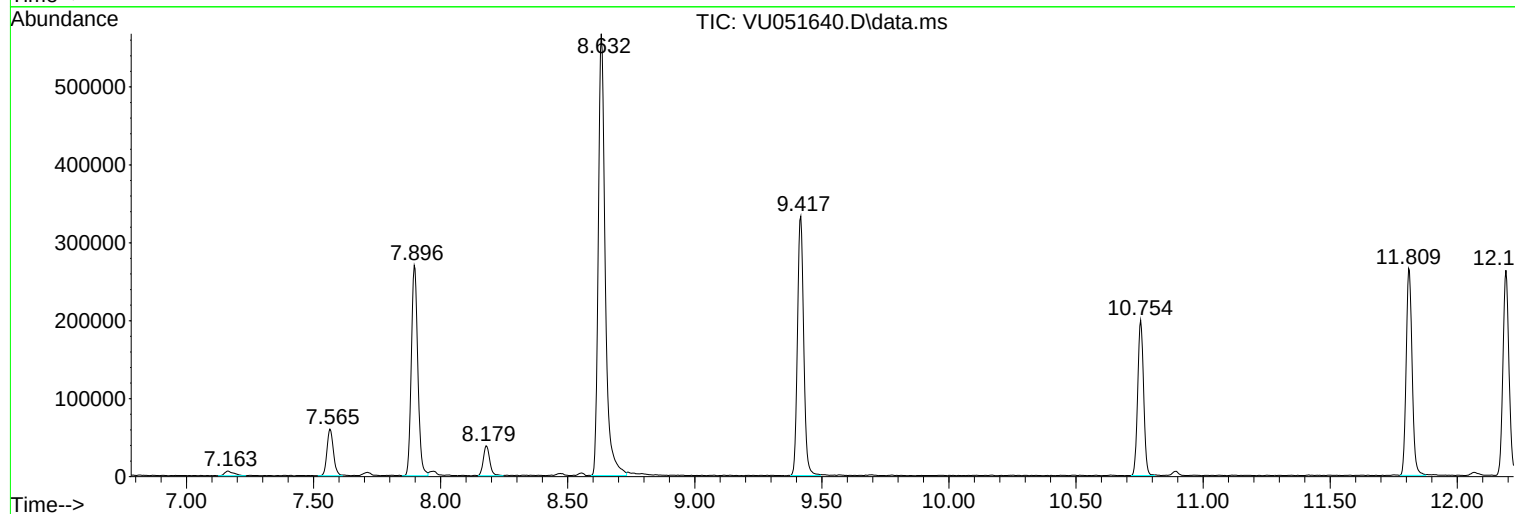
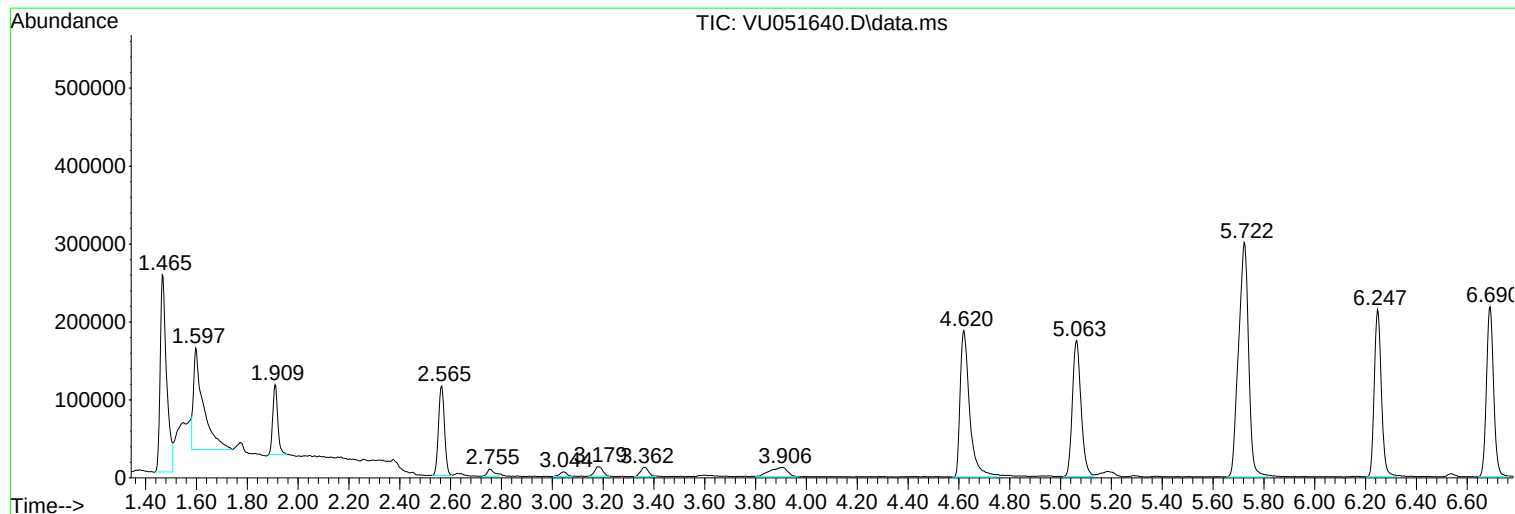
Sum of corrected areas: 7416038

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU103122\
Data File : VU051640.D
Acq On : 01 Nov 2022 03:41
Operator : JC/MD
Sample : N5319-17
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHAB2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU103122\
Data File : VU051640.D
Acq On : 01 Nov 2022 03:41
Operator : JC/MD
Sample : N5319-17
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHAB2

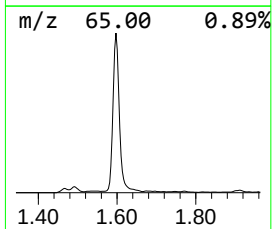
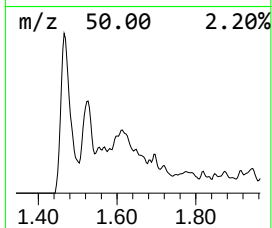
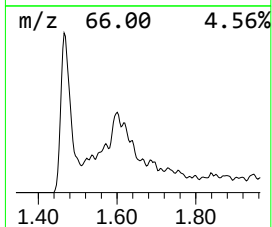
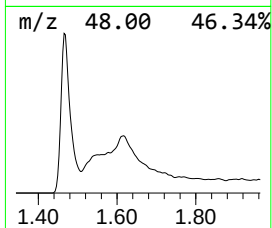
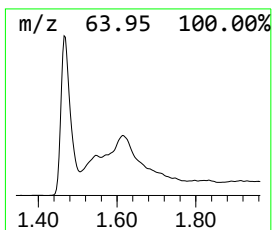
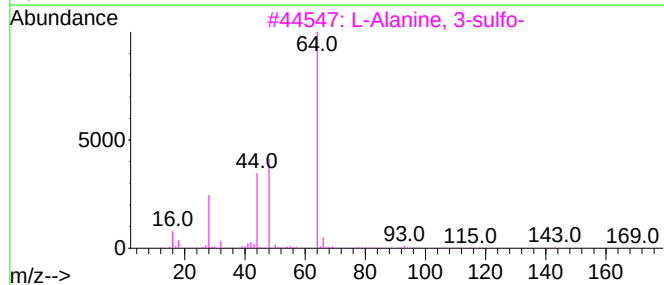
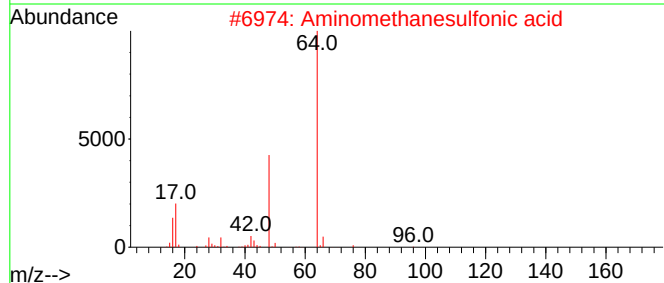
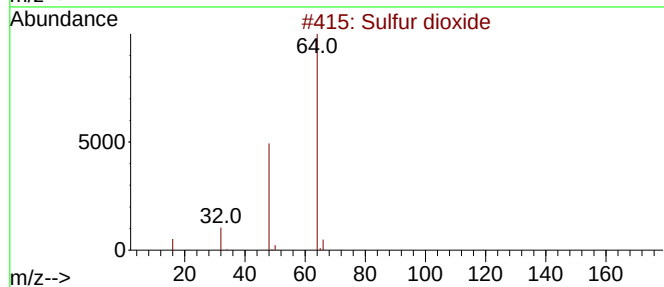
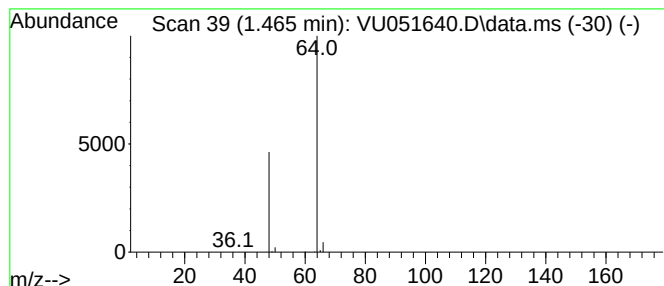
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
1.465	5.36 ug/L	446394	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	4



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU103122\
Data File : VU051640.D
Acq On : 01 Nov 2022 03:41
Operator : JC/MD
Sample : N5319-17
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHAB2

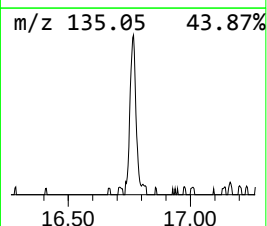
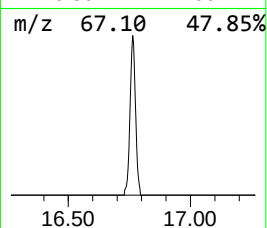
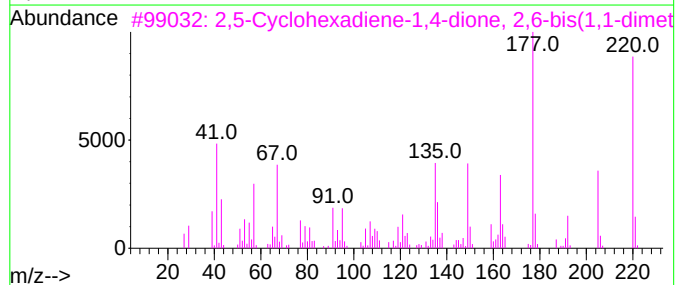
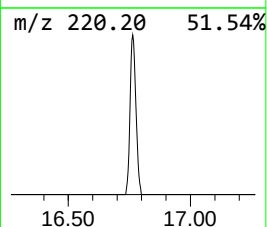
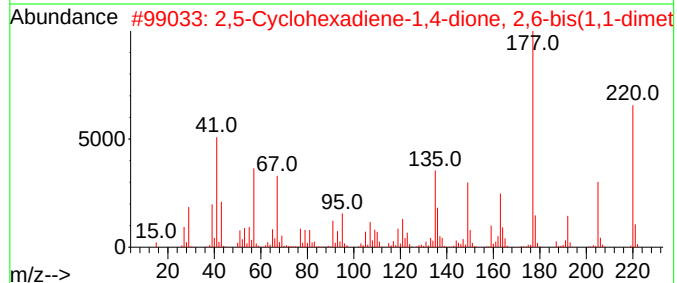
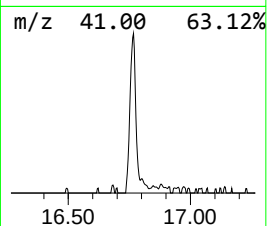
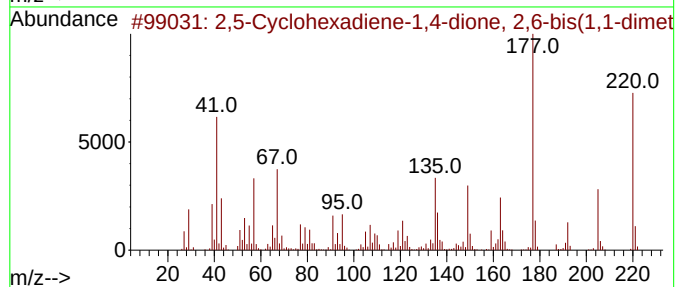
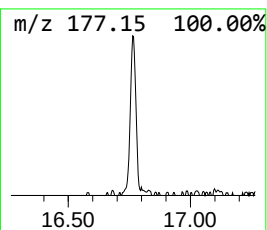
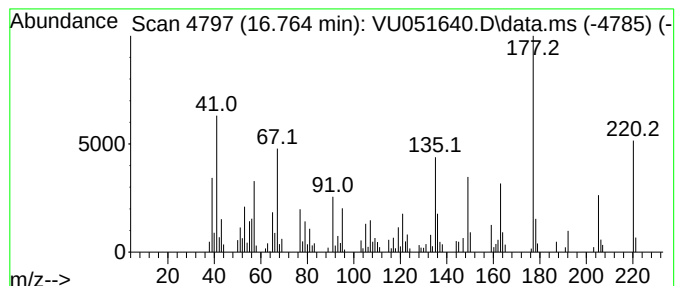
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.764	1.20 ug/L	103769	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	99
2			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	99
3			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	99
4			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94
5			.beta.-Oplophenone	220	C15H24O	028305-60-4	49



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU103122\
Data File : VU051640.D
Acq On : 01 Nov 2022 03:41
Operator : JC/MD
Sample : N5319-17
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHAB2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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	1.465	5.4	ug/L	446394	1	6.247	416341	5.0
2,5-Cyclohexadi...	16.764	1.2	ug/L	103769	3	11.809	433120	5.0