

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111424\
 Data File : VU061675.D
 Acq On : 14 Nov 2024 16:33
 Operator : MD/SY
 Sample : P4804-10DL 5X
 Misc : 25mL/MSVOA_U/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 H46T8DL

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\SFAMUTR111324WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU061675.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.489	55	62	67	rBV2	8243	8834	1.09%	0.125%
2	1.596	86	95	107	rBV2	105014	137617	16.97%	1.943%
3	1.724	117	135	141	rBV3	16903	55495	6.84%	0.783%
4	1.911	185	193	207	rBV	66217	112013	13.81%	1.581%
5	2.554	381	393	414	rVB	141941	232292	28.65%	3.279%
6	3.174	573	586	605	rVB	14794	34598	4.27%	0.488%
7	3.354	627	642	665	rBV3	54954	130477	16.09%	1.842%
8	3.686	731	745	765	rBV	35671	79607	9.82%	1.124%
9	4.650	1024	1045	1079	rBV3	274072	762067	93.99%	10.758%
10	5.052	1156	1170	1199	rBV	118569	269403	33.23%	3.803%
11	5.714	1356	1376	1410	rBV2	257943	671311	82.79%	9.477%
12	6.238	1521	1539	1561	rBV	218705	426844	52.64%	6.026%
13	6.531	1616	1630	1664	rBV	416699	810828	100.00%	11.446%
14	6.679	1664	1676	1699	rVB	148336	297437	36.68%	4.199%
15	7.560	1939	1950	1983	rBV	66553	126661	15.62%	1.788%
16	7.891	2040	2053	2078	rBV	318698	572512	70.61%	8.082%
17	8.174	2130	2141	2164	rBV	37959	69286	8.55%	0.978%
18	8.547	2248	2257	2268	rVB2	13915	23410	2.89%	0.330%
19	8.644	2273	2287	2329	rBV	259610	598125	73.77%	8.443%
20	9.412	2513	2526	2556	rBV	301482	534796	65.96%	7.549%
21	10.753	2928	2943	2959	rBV	112199	187072	23.07%	2.641%
22	11.804	3259	3270	3291	rBV	289090	479578	59.15%	6.770%
23	12.187	3375	3389	3419	rBV	277202	463640	57.18%	6.545%

Sum of corrected areas: 7083903

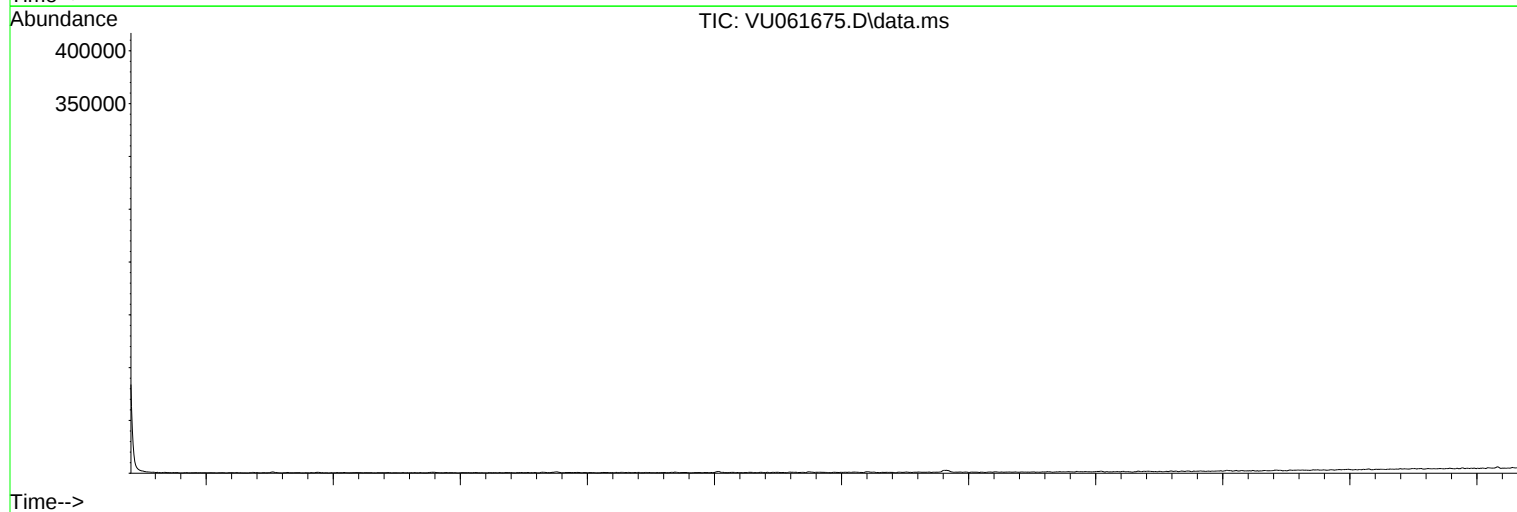
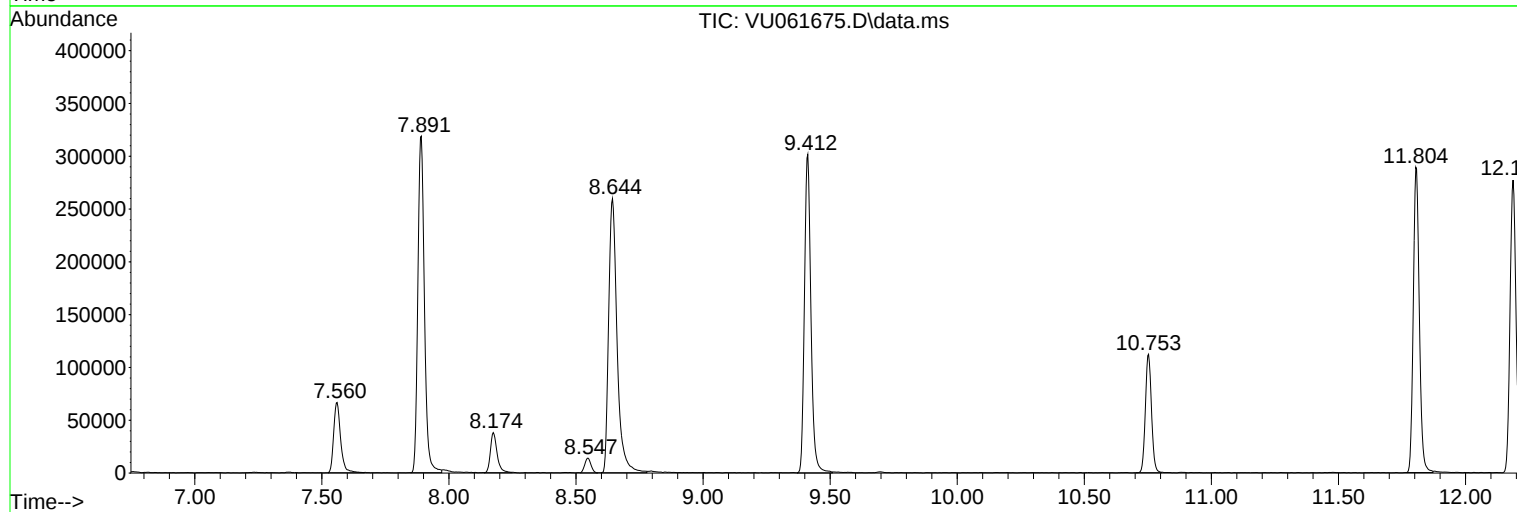
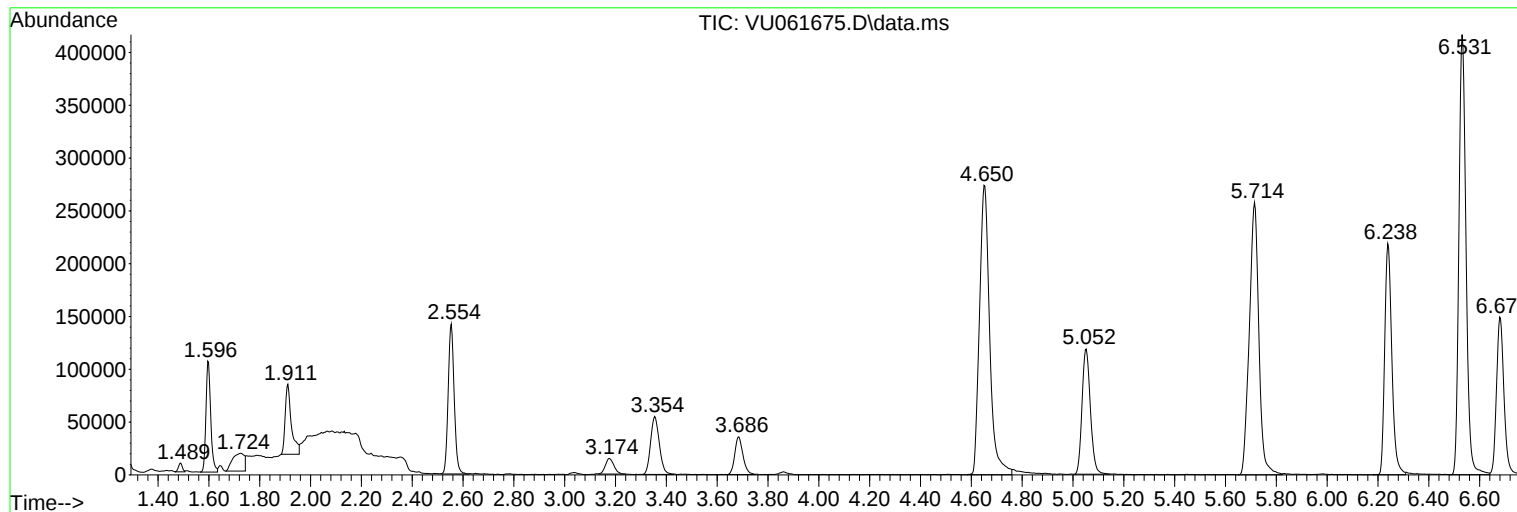
Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111424\
Data File : VU061675.D
Acq On : 14 Nov 2024 16:33
Operator : MD/SY
Sample : P4804-10DL 5X
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
H46T8DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111324WMA.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\VU111424\
Data File : VU061675.D
Acq On : 14 Nov 2024 16:33
Operator : MD/SY
Sample : P4804-10DL 5X
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
H46T8DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111324WMA.M
Quant Title : TRACE VOA SFAM1.0

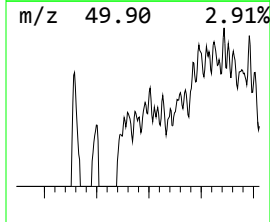
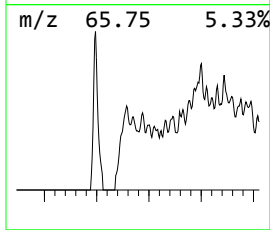
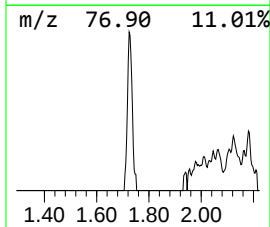
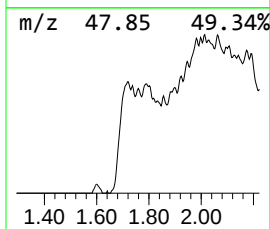
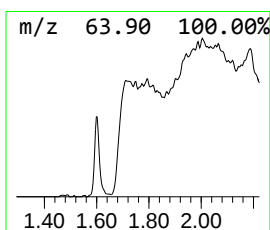
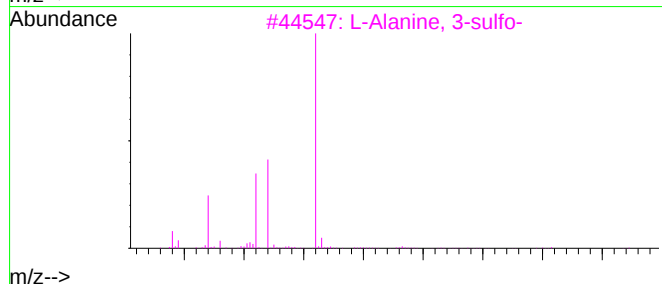
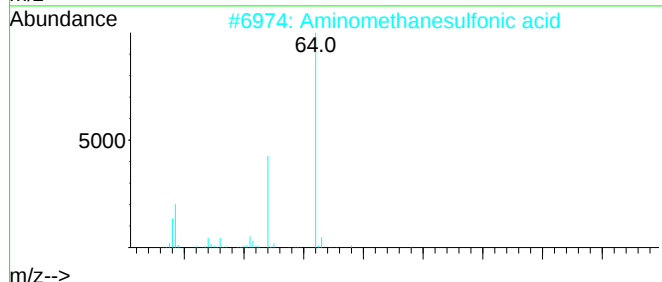
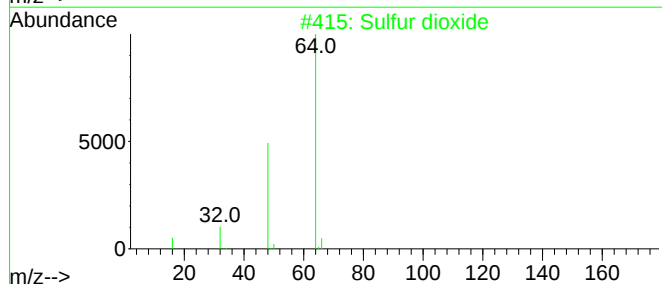
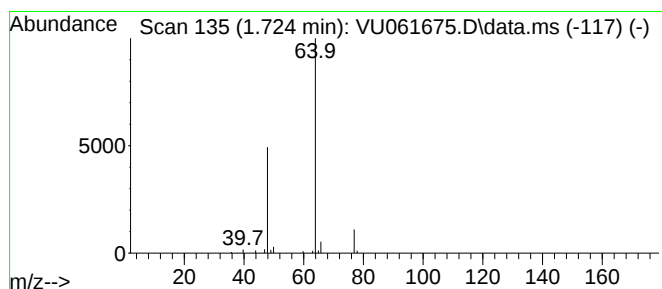
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.724	0.65 ug/L	55495	1,4-Difluorobenzene	6.238

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	64
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	Sulfur dioxide	64	O2S	007446-09-5	5



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111424\
Data File : VU061675.D
Acq On : 14 Nov 2024 16:33
Operator : MD/SY
Sample : P4804-10DL 5X
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
H46T8DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111324WMA.M
Quant Title : TRACE VOA SFAM1.0

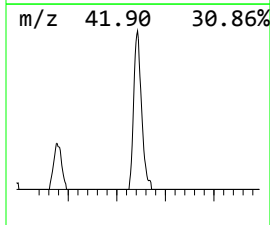
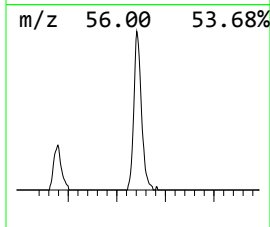
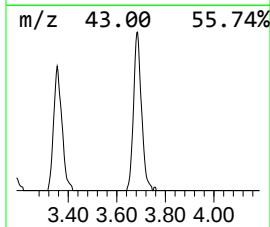
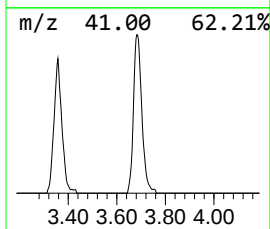
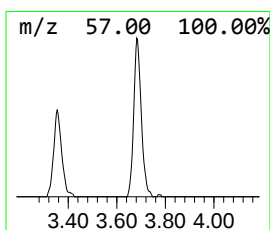
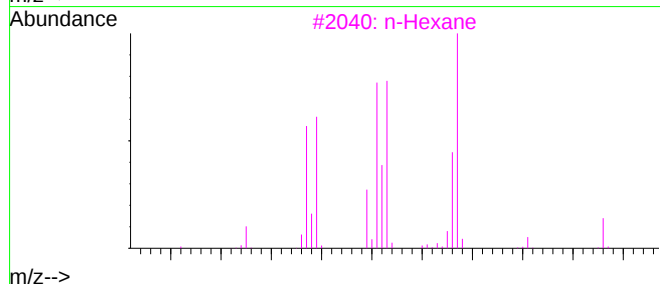
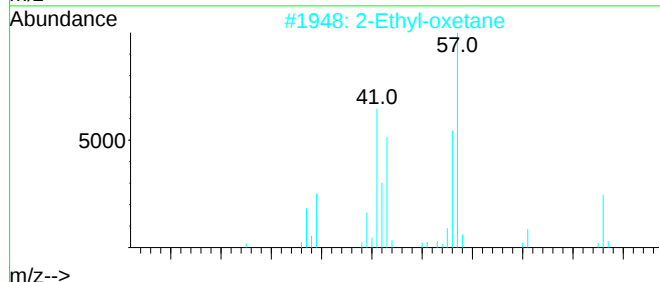
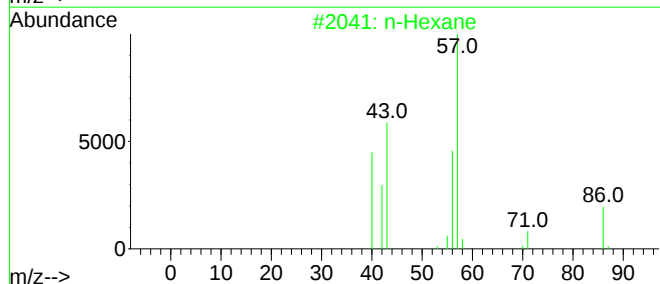
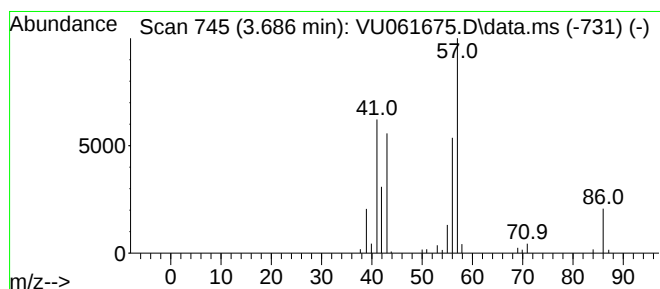
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.686	0.93 ug/L	79607	1,4-Difluorobenzene	6.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	86
2	2-Ethyl-oxetane	86	C5H10O	1010386-40-2	80
3	n-Hexane	86	C6H14	000110-54-3	56
4	n-Hexane	86	C6H14	000110-54-3	50
5	Pentane, 3-methyl-	86	C6H14	000096-14-0	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111424\
Data File : VU061675.D
Acq On : 14 Nov 2024 16:33
Operator : MD/SY
Sample : P4804-10DL 5X
Misc : 25mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
H46T8DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111324WMA.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	1.724	0.7	ug/L	55495	1	6.238	426844	5.0
(DEL) Alkane: S...	3.686	0.9	ug/L	79607	1	6.238	426844	5.0