

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV071222\
 Data File : VV026733.D
 Acq On : 12 Jul 2022 18:14
 Operator : SY/MD
 Sample : N3601-16
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DBUA7

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_V\Method\SFAMVTR071122WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV026733.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.298	75	80	100	rVB	171261	196258	20.04%	2.065%
2	1.423	102	119	122	rBV	63230	168904	17.24%	1.777%
3	1.561	156	162	174	rVB	144316	170445	17.40%	1.793%
4	2.098	320	329	351	rVB	301192	465237	47.50%	4.895%
5	2.198	352	360	377	rVV	22856	39190	4.00%	0.412%
6	2.285	377	387	400	rVB	52205	80541	8.22%	0.847%
7	3.908	880	892	938	rBV2	79485	351186	35.86%	3.695%
8	4.342	1010	1027	1052	rBV	171173	435089	44.42%	4.578%
9	5.043	1229	1245	1284	rBV3	372309	979461	100.00%	10.305%
10	5.365	1333	1345	1365	rBV3	14587	33243	3.39%	0.350%
11	5.613	1411	1422	1458	rBV	254183	530082	54.12%	5.577%
12	5.912	1500	1515	1539	rBV	138771	287644	29.37%	3.026%
13	6.066	1550	1563	1590	rBV	216631	453945	46.35%	4.776%
14	6.985	1838	1849	1869	rBV2	68687	133990	13.68%	1.410%
15	7.313	1939	1951	1970	rBV	388703	682030	69.63%	7.176%
16	7.522	2006	2016	2033	rBV	44494	81127	8.28%	0.854%
17	7.625	2038	2048	2065	rBV	38392	71409	7.29%	0.751%
18	7.973	2135	2156	2180	rBV	403436	686747	70.11%	7.225%
19	8.092	2182	2193	2221	rBV	407797	799486	81.63%	8.412%
20	8.850	2418	2429	2455	rBV	405772	759241	77.52%	7.988%
21	9.018	2472	2481	2491	rBV2	6396	11074	1.13%	0.117%
22	9.146	2502	2521	2539	rVB4	18557	44377	4.53%	0.467%
23	9.500	2622	2631	2638	rBV4	8250	12407	1.27%	0.131%
24	9.545	2638	2645	2657	rVB	14785	23707	2.42%	0.249%
25	10.214	2843	2853	2870	rBV	164613	268859	27.45%	2.829%
26	10.381	2891	2905	2914	rBV6	4507	10443	1.07%	0.110%
27	10.452	2918	2927	2938	rBV5	7052	12711	1.30%	0.134%
28	10.542	2943	2955	2962	rBV4	9924	16331	1.67%	0.172%
29	10.741	3007	3017	3024	rBV	6454	10380	1.06%	0.109%
30	10.918	3061	3072	3080	rBV	16808	24907	2.54%	0.262%
31	11.249	3163	3175	3195	rBV	383044	635787	64.91%	6.689%
32	11.339	3195	3203	3215	rVB5	15871	31534	3.22%	0.332%
33	11.529	3251	3262	3280	rBV	91202	170087	17.37%	1.790%
34	11.622	3280	3291	3315	rVB	403986	684728	69.91%	7.204%
35	12.468	3544	3554	3563	rVB3	6535	10500	1.07%	0.110%
36	12.879	3676	3682	3691	rVV5	12107	16809	1.72%	0.177%

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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_V\Method\SFAMVTR071122WMA.M
Title : TRACE VOA SFAM1.0

37	12.950	3695	3704	3714	rVB5	7904	12963	1.32%	0.136%
38	13.271	3795	3804	3811	rBV8	7798	12933	1.32%	0.136%
39	13.503	3865	3876	3885	rBV2	21039	34586	3.53%	0.364%
40	14.635	4217	4228	4236	rBV2	14296	22399	2.29%	0.236%
41	14.818	4277	4285	4299	rVB3	11028	20820	2.13%	0.219%
42	15.808	4585	4593	4600	rBV7	6963	11015	1.12%	0.116%

Sum of corrected areas: 9504612

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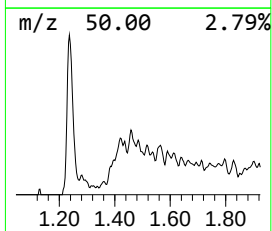
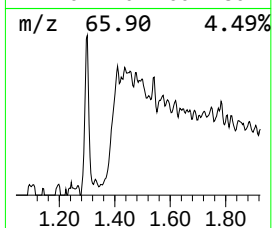
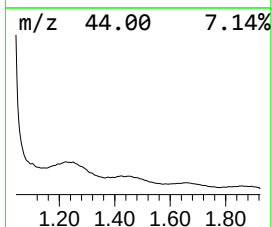
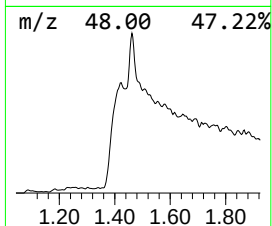
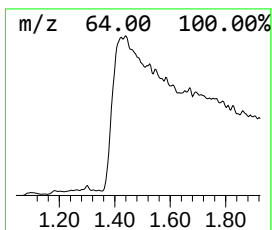
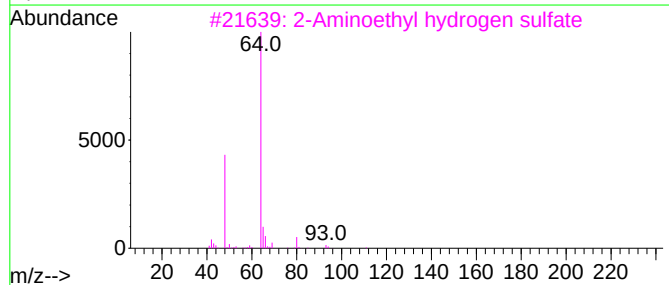
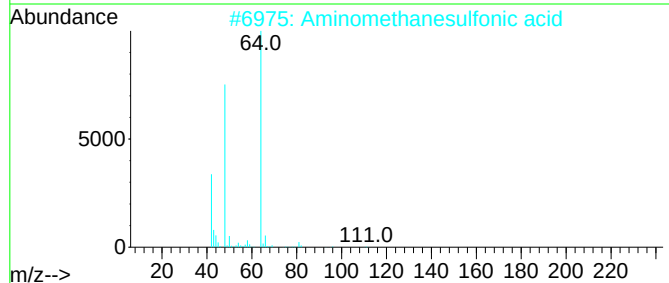
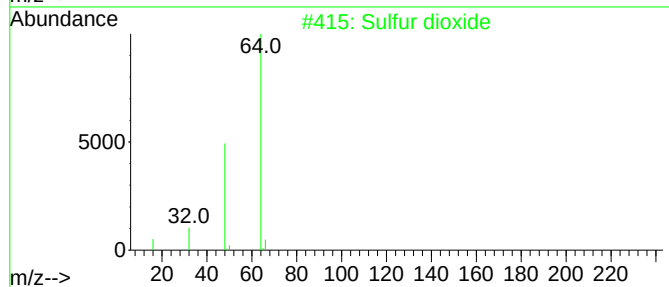
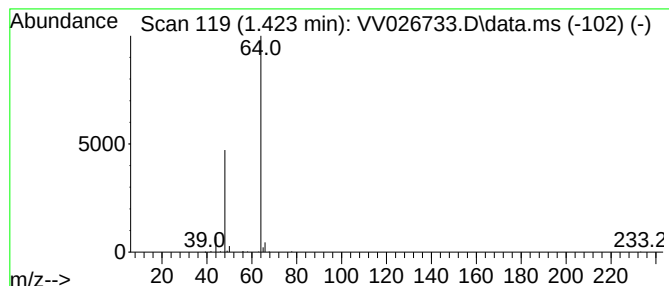
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR071122WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
1.423	1.59 ug/L	168904	1,4-Difluorobenzene	5.613

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	83
3			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
5			Dibenzo[cd,g]indazole-3-sulfonic...	300	C14H8N2O4S	293765-87-4	64



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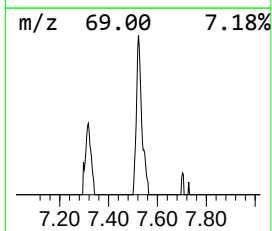
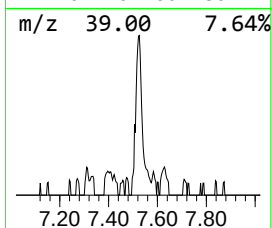
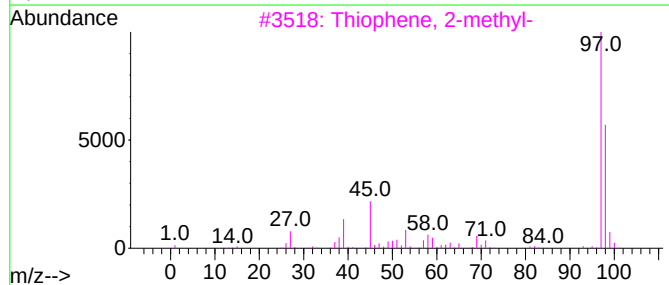
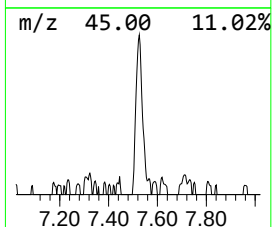
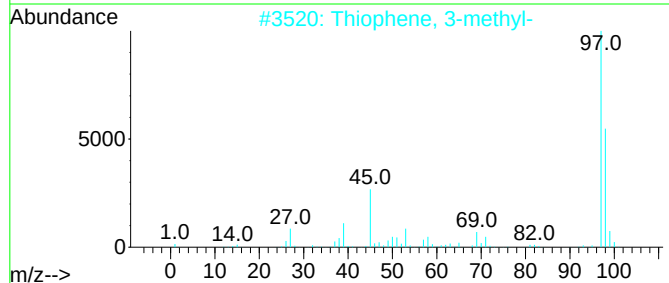
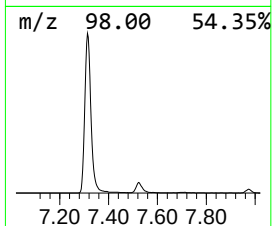
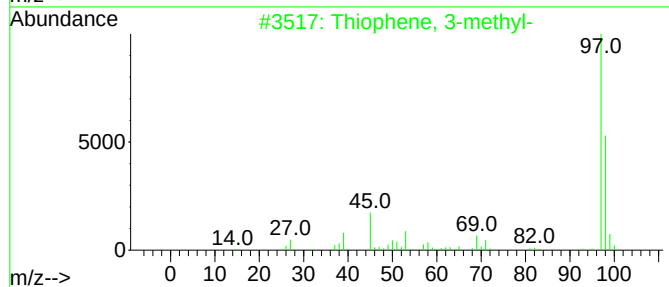
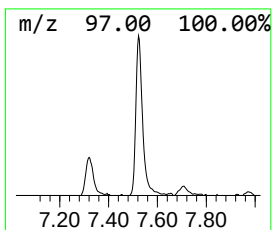
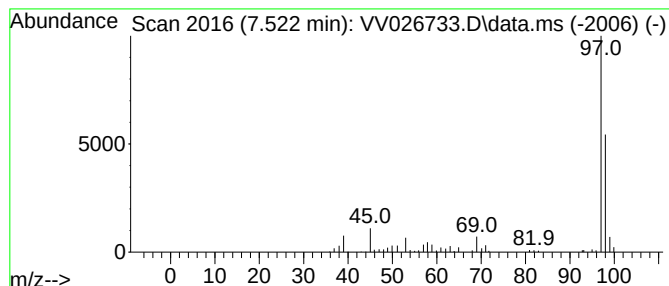
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR071122WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Thiophene, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.522	0.53 ug/L	81127	Chlorobenzene-d5	8.850

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, 3-methyl-	98	C5H6S	000616-44-4	91
2			Thiophene, 3-methyl-	98	C5H6S	000616-44-4	91
3			Thiophene, 2-methyl-	98	C5H6S	000554-14-3	91
4			Thiophene, 2-methyl-	98	C5H6S	000554-14-3	91
5			Thiophene, 2-methyl-	98	C5H6S	000554-14-3	91



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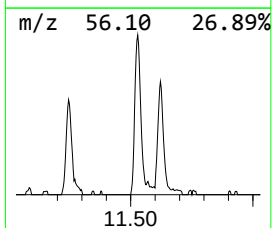
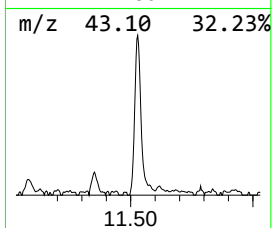
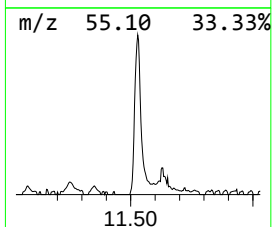
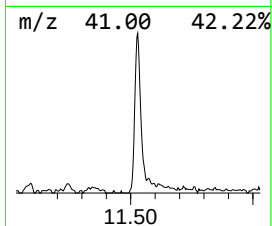
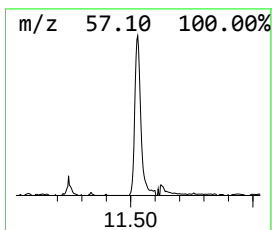
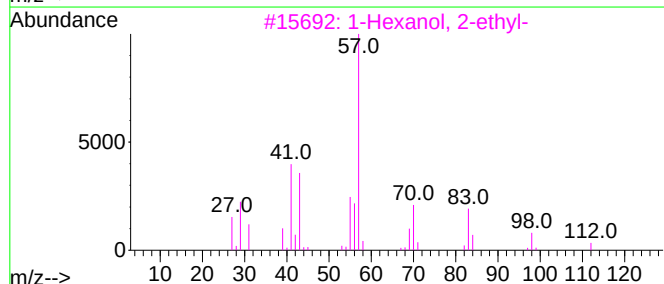
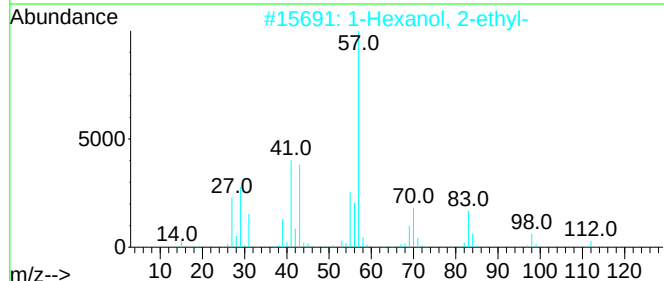
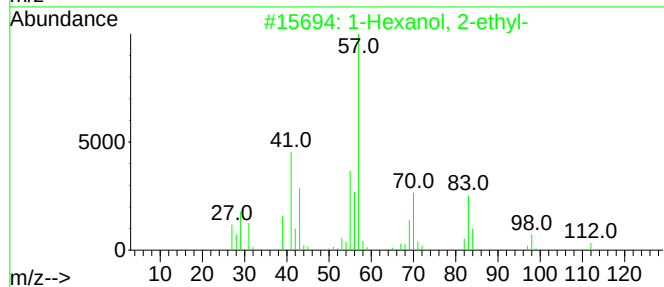
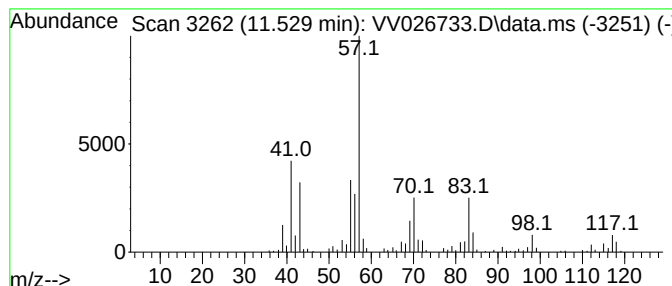
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.529	1.34 ug/L	170087	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	86
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	80
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	80
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
5	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR071122WMA.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	1.423	1.6	ug/L	168904	1	5.613	530082	5.0
Thiophene, 3-me...	7.522	0.5	ug/L	81127	2	8.850	759241	5.0
1-Hexanol, 2-et...	11.529	1.3	ug/L	170087	3	11.249	635787	5.0