

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101124\
 Data File : VU061113.D
 Acq On : 11 Oct 2024 13:00
 Operator : MD/SY
 Sample : P4380-21
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E27G6

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\SFAMUTR100124WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU061113.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.367	16	24	38	rBV2	36756	44822	5.88%	0.683%
2	1.483	45	60	61	rBV3	17422	31399	4.12%	0.479%
3	1.496	62	64	70	rVB	12939	11032	1.45%	0.168%
4	1.608	88	99	110	rBV2	90152	122138	16.04%	1.862%
5	1.744	132	141	159	rVB	331171	417136	54.77%	6.359%
6	1.930	190	199	215	rBV	61446	105028	13.79%	1.601%
7	2.010	218	224	231	rVB	14559	18097	2.38%	0.276%
8	2.075	235	244	255	rBV2	9334	26431	3.47%	0.403%
9	2.213	283	287	298	rVB	17543	24199	3.18%	0.369%
10	2.412	340	349	370	rVB2	22196	54650	7.18%	0.833%
11	2.573	389	399	410	rVB	101402	160339	21.05%	2.444%
12	4.734	1046	1071	1116	rBV3	40058	226800	29.78%	3.457%
13	5.091	1167	1182	1207	rVB	90712	210245	27.60%	3.205%
14	5.759	1372	1390	1419	rBV2	200932	496845	65.23%	7.574%
15	6.277	1539	1551	1574	rBV	193666	365669	48.01%	5.574%
16	6.714	1674	1687	1704	rBV	121011	233392	30.64%	3.558%
17	7.579	1944	1956	1971	rBV	65197	115761	15.20%	1.765%
18	7.907	2046	2058	2076	rBV	232740	414053	54.36%	6.312%
19	7.984	2078	2082	2095	rVB2	6775	10079	1.32%	0.154%
20	8.190	2135	2146	2163	rBV2	38029	67501	8.86%	1.029%
21	8.560	2252	2261	2271	rVB2	11754	18597	2.44%	0.283%
22	8.644	2275	2287	2326	rBV	270996	551721	72.44%	8.411%
23	9.418	2516	2528	2561	rVB	267459	452172	59.37%	6.893%
24	10.753	2930	2943	2961	rBV	85173	140258	18.41%	2.138%
25	11.084	3038	3046	3055	rBV	7752	11842	1.55%	0.181%
26	11.807	3258	3271	3288	rBV	278221	454486	59.67%	6.928%
27	12.055	3336	3348	3378	rBV	71313	183320	24.07%	2.795%
28	12.187	3378	3389	3414	rVV	229185	382941	50.28%	5.838%
29	12.315	3417	3429	3439	rVV9	4991	9621	1.26%	0.147%
30	12.875	3594	3603	3613	rVB6	4482	9007	1.18%	0.137%
31	13.020	3639	3648	3657	rVB	12863	20527	2.70%	0.313%
32	13.280	3722	3729	3738	rBV2	6333	9865	1.30%	0.150%
33	13.444	3772	3780	3798	rVB5	8232	14572	1.91%	0.222%
34	13.833	3890	3901	3916	rBV4	31974	70924	9.31%	1.081%
35	14.077	3964	3977	4005	rVV	458642	761651	100.00%	11.611%
36	14.203	4005	4016	4028	rVB	8387	14188	1.86%	0.216%

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Title : TRACE VOA SFAM1.0

37	14.878	4218	4226	4236	rVB6	5523	9180	1.21%	0.140%
38	15.216	4318	4331	4344	rBV	52529	85765	11.26%	1.307%
39	15.405	4378	4390	4401	rBV	34111	55445	7.28%	0.845%
40	15.949	4552	4559	4565	rBV2	11154	15037	1.97%	0.229%
41	15.994	4567	4573	4583	rVB3	7791	11606	1.52%	0.177%
42	16.261	4647	4656	4666	rBV3	8977	14256	1.87%	0.217%
43	16.402	4690	4700	4707	rBV	19394	30986	4.07%	0.472%
44	16.441	4707	4712	4723	rVB3	10315	16147	2.12%	0.246%
45	16.878	4839	4848	4858	rBV5	18015	32684	4.29%	0.498%
46	17.090	4907	4914	4928	rVB3	8325	13993	1.84%	0.213%
47	17.408	5007	5013	5022	rVB	8457	13416	1.76%	0.205%

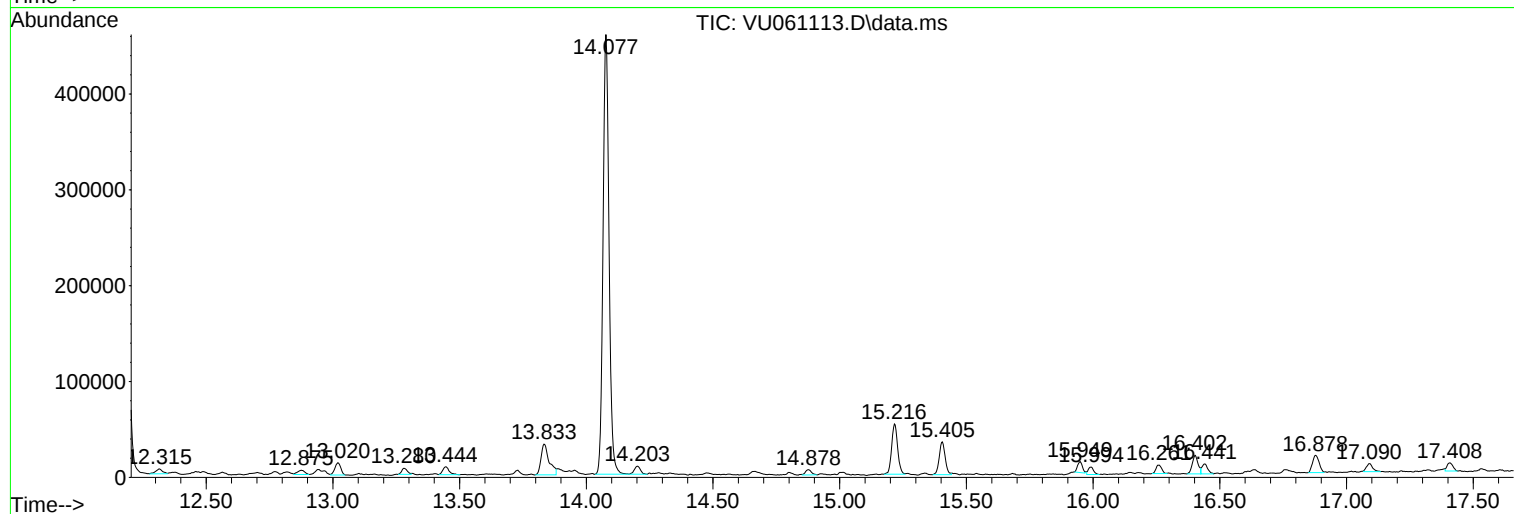
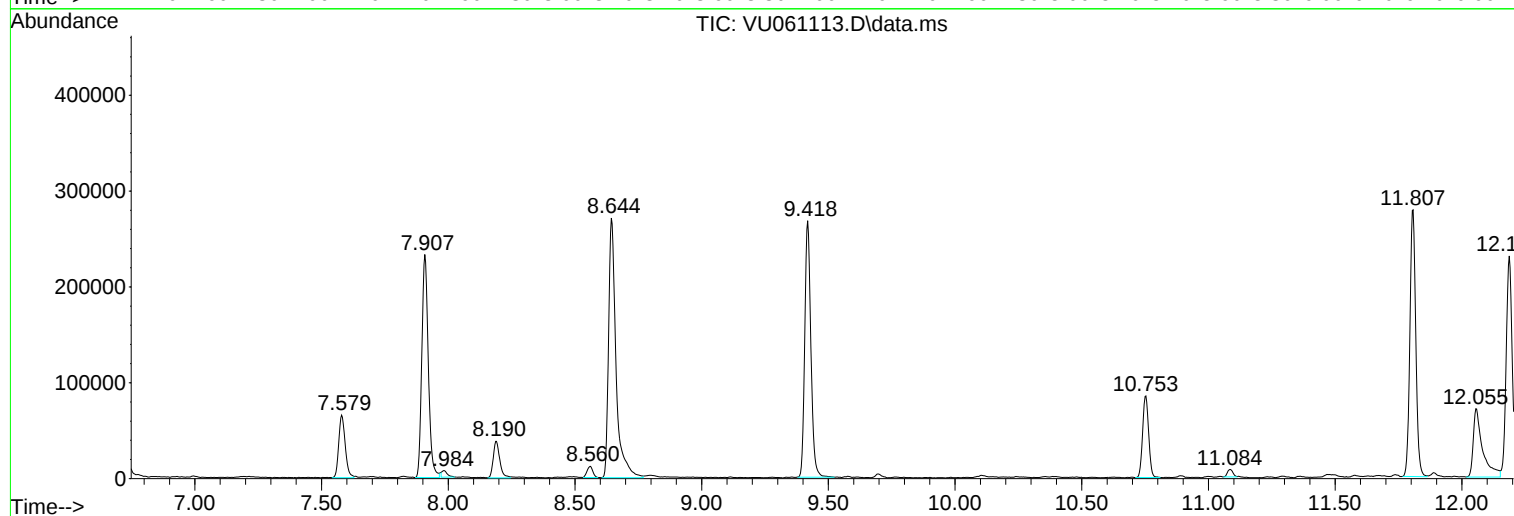
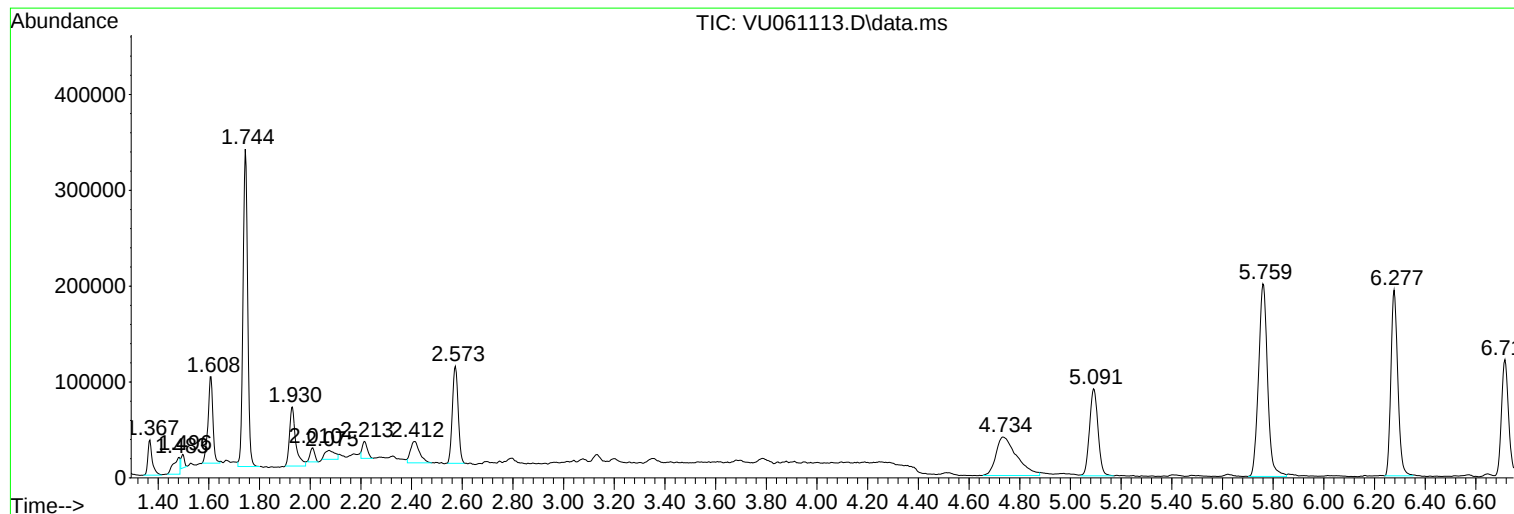
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ClientSampleId :
E27G6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100124WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Instrument :
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ClientSampleId :
E27G6

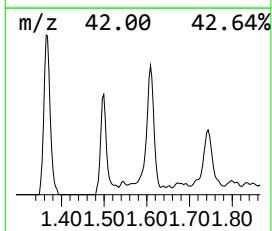
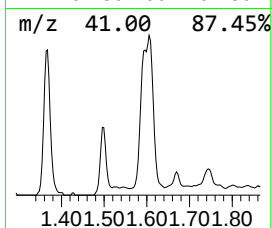
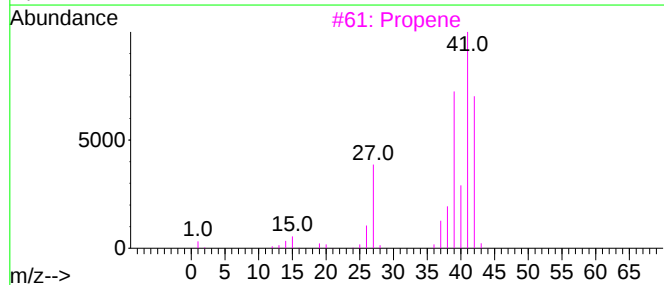
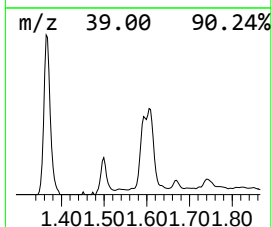
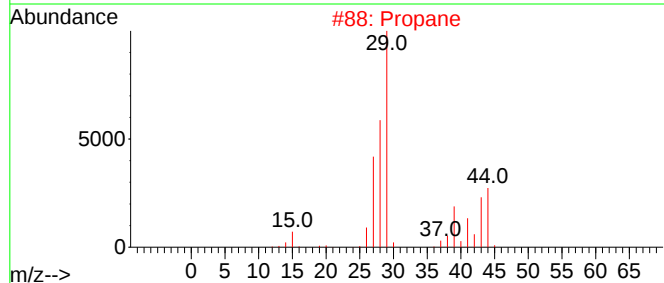
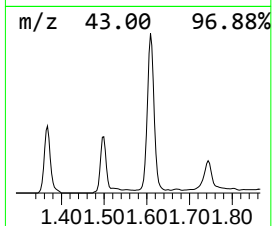
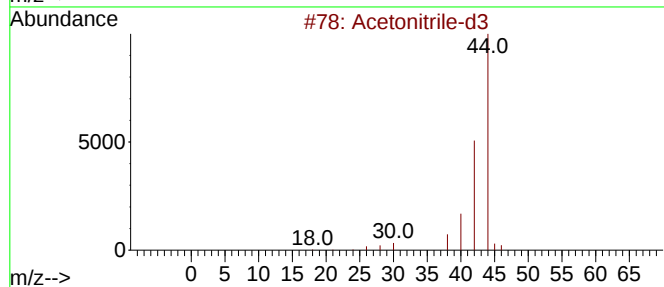
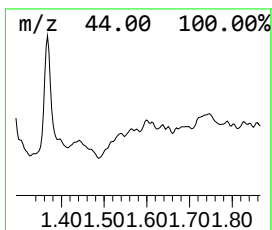
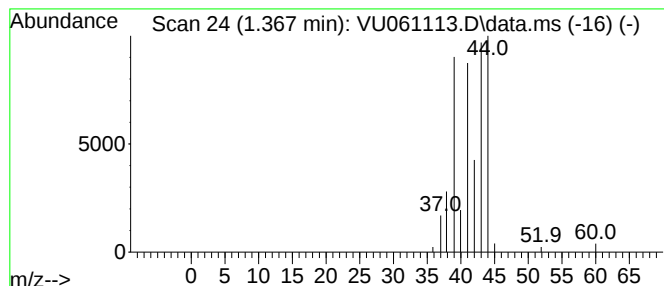
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.367	0.61 ug/L	44822	1,4-Difluorobenzene	6.277

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetonitrile-d3	44	C2D3N	002206-26-0	9
2			Propane	44	C3H8	000074-98-6	9
3			Propene	42	C3H6	000115-07-1	9
4			Acetonitrile-d3	44	C2D3N	002206-26-0	4
5			Propane	44	C3H8	000074-98-6	4



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E27G6

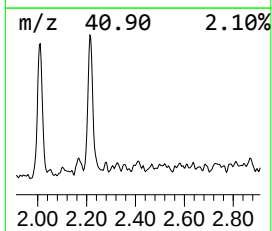
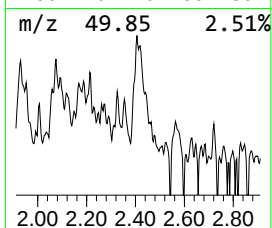
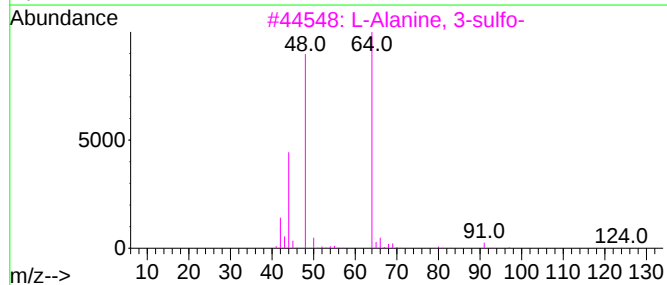
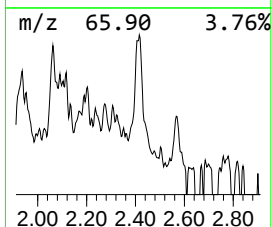
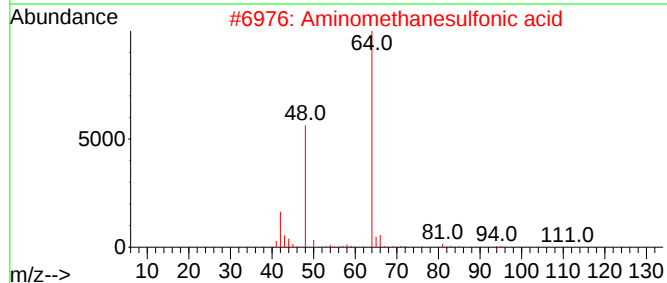
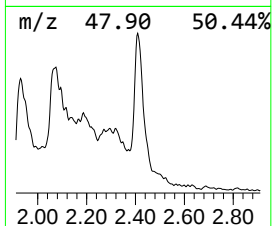
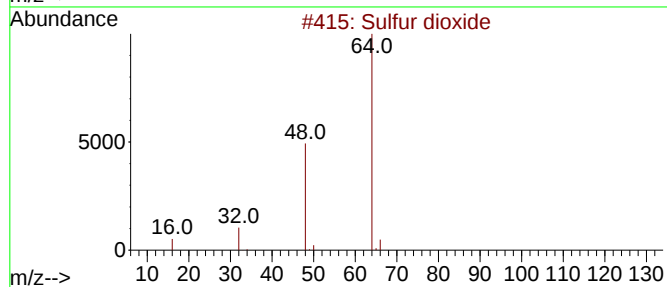
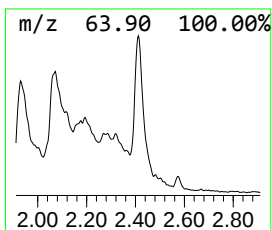
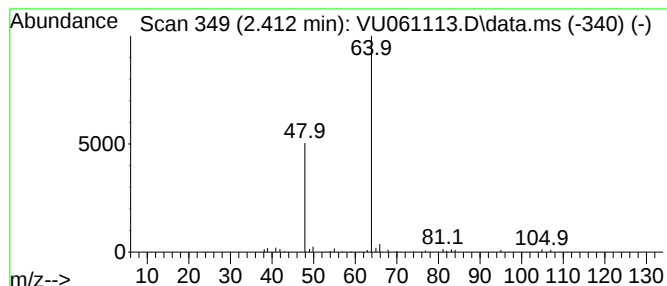
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100124WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Sulfur dioxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.412	0.75 ug/L	54650	1,4-Difluorobenzene	6.277

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	74
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\VU101124\
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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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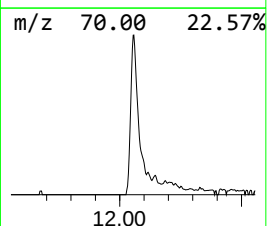
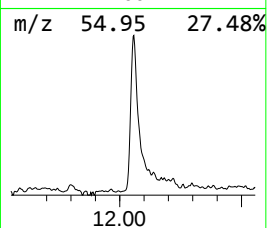
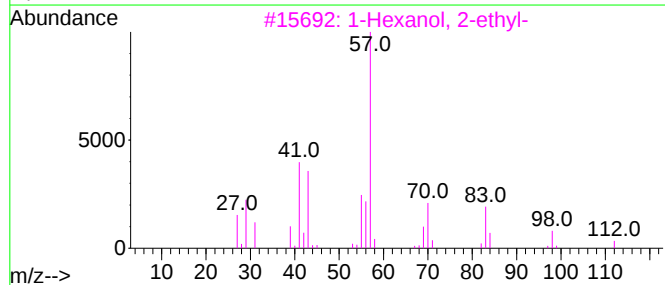
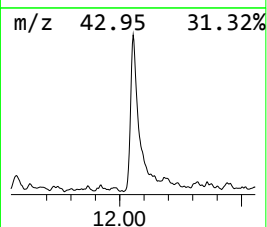
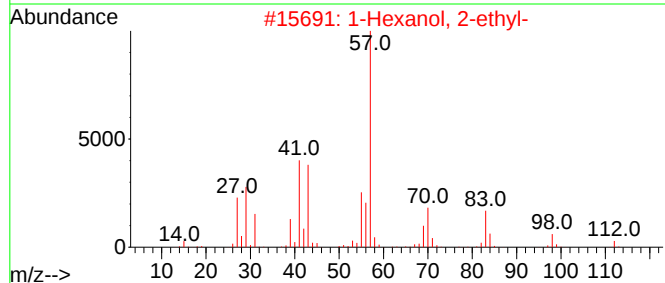
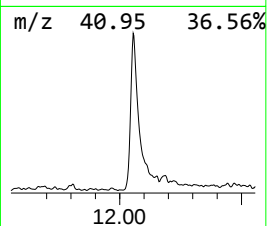
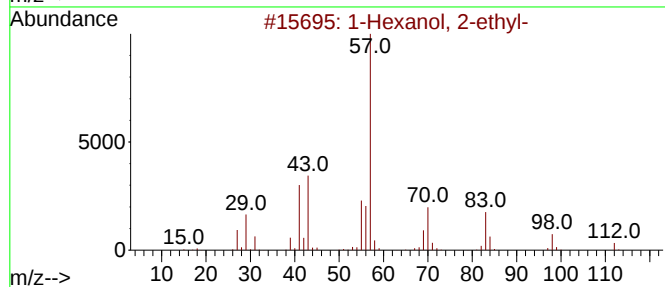
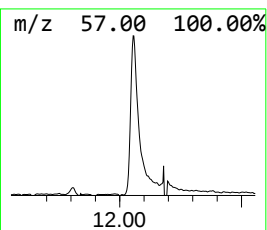
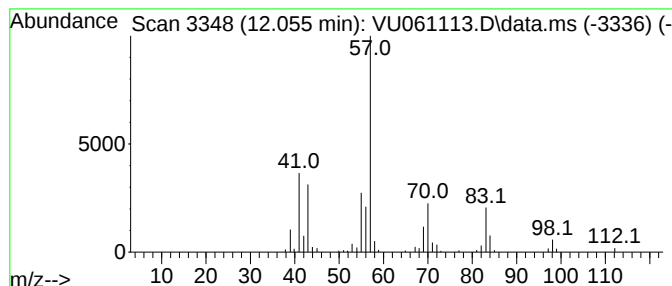
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100124WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.055	2.02 ug/L	183320	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59



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ClientSampleId :
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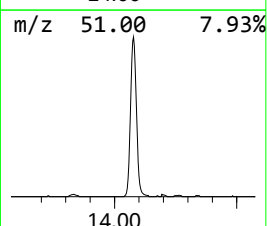
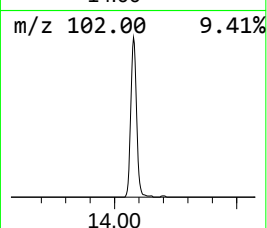
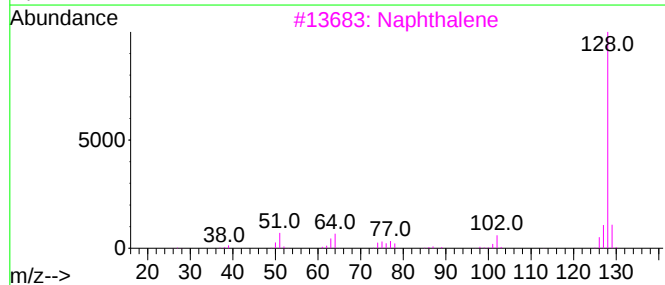
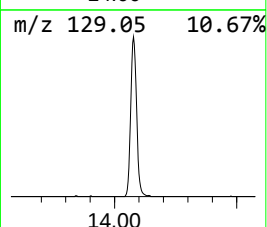
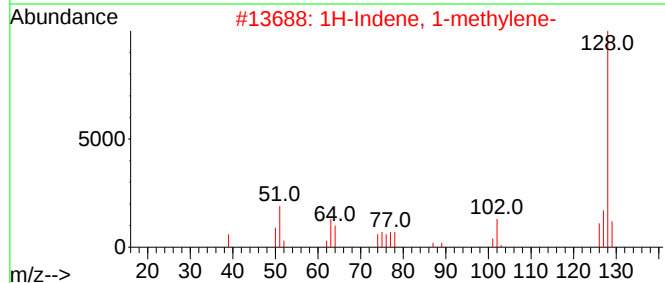
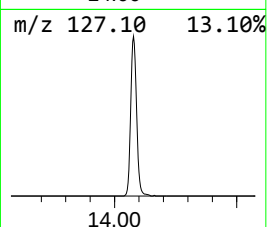
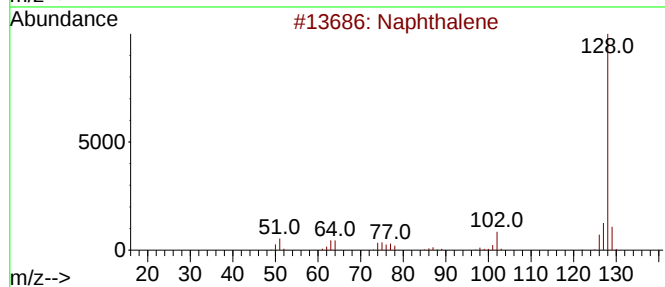
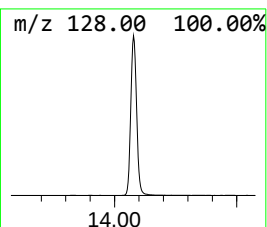
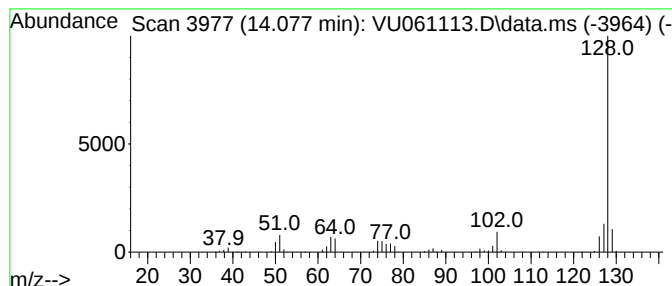
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100124WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.077	8.38 ug/L	761651	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	95
3			Naphthalene	128	C10H8	000091-20-3	94
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	91



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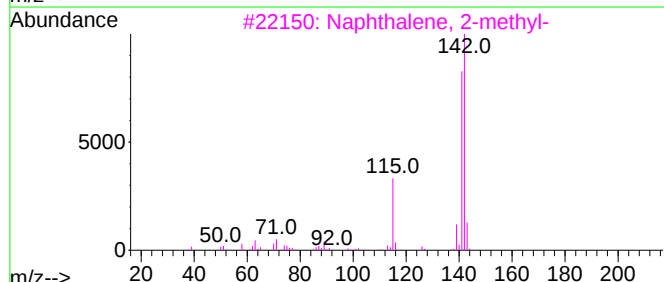
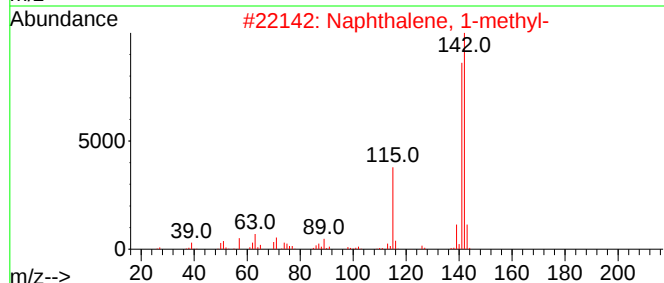
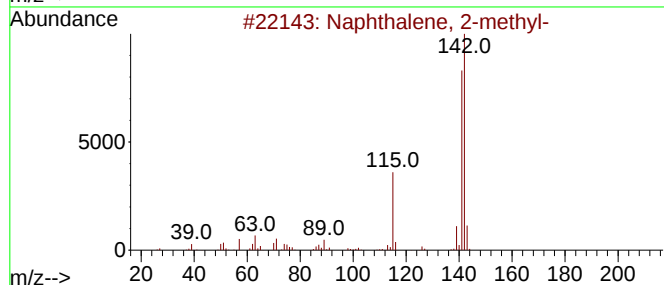
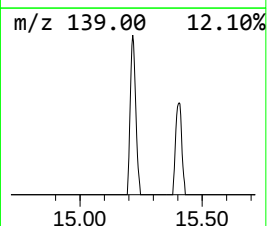
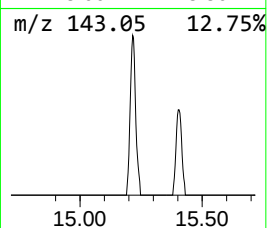
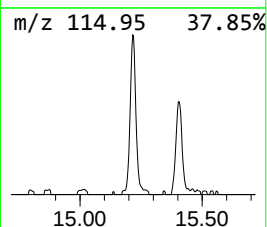
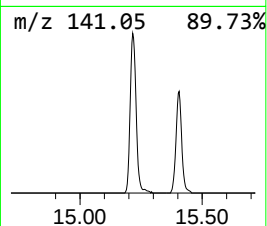
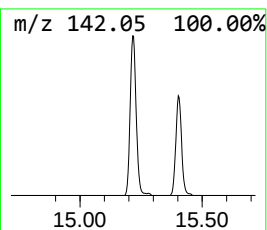
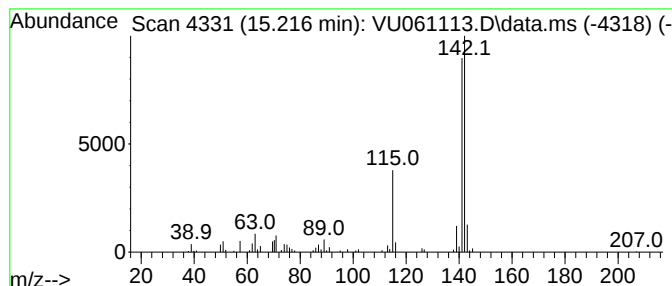
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100124WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 1H-Indene, 1-ethylidene- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.216	0.94 ug/L	85765	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
4			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	95
5			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101124\
Data File : VU061113.D
Acq On : 11 Oct 2024 13:00
Operator : MD/SY
Sample : P4380-21
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E27G6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100124WMA.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
unknown-01	1.367	0.6	ug/L	44822	1	6.277	365669	5.0
Sulfur dioxide	2.412	0.8	ug/L	54650	1	6.277	365669	5.0
1-Hexanol, 2-et...	12.055	2.0	ug/L	183320	3	11.807	454486	5.0
Azulene	14.077	8.4	ug/L	761651	3	11.807	454486	5.0
1H-Indene, 1-et...	15.216	0.9	ug/L	85765	3	11.807	454486	5.0