

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU091223\
 Data File : VU055250.D
 Acq On : 12 Sep 2023 16:03
 Operator : MD/SY
 Sample : 04350-01
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH4J5

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\SFAMUTR090123WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU055250.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.464	47	54	65	rVB	54532	58933	7.64%	0.855%
2	1.595	88	95	106	rVB	44375	48802	6.32%	0.708%
3	1.821	145	165	175	rBV2	19609	58130	7.53%	0.843%
4	1.907	184	192	206	rVB	62779	82561	10.70%	1.197%
5	2.377	328	338	352	rVB5	9739	18059	2.34%	0.262%
6	2.566	384	397	412	rBV3	106519	202532	26.25%	2.937%
7	3.357	632	643	661	rVB8	8348	19330	2.51%	0.280%
8	4.663	1026	1049	1074	rBV2	243121	771589	100.00%	11.190%
9	5.062	1156	1173	1206	rVB3	113447	285392	36.99%	4.139%
10	5.521	1303	1316	1329	rBV3	16877	38143	4.94%	0.553%
11	5.724	1359	1379	1395	rBV4	212224	554032	71.80%	8.035%
12	6.248	1529	1542	1569	rBV	236056	456529	59.17%	6.621%
13	6.541	1619	1633	1654	rBV	359217	684476	88.71%	9.926%
14	6.688	1665	1679	1697	rVB2	146037	286862	37.18%	4.160%
15	7.566	1940	1952	1968	rBV2	49718	91468	11.85%	1.326%
16	7.897	2039	2055	2073	rBV	246262	434351	56.29%	6.299%
17	8.180	2132	2143	2160	rBV2	28343	50807	6.58%	0.737%
18	8.550	2247	2258	2273	rBV	137975	236033	30.59%	3.423%
19	8.634	2273	2284	2324	rVV2	288472	657784	85.25%	9.539%
20	9.415	2514	2527	2551	rBV	365980	632435	81.97%	9.172%
21	10.753	2932	2943	2960	rBV	107581	176296	22.85%	2.557%
22	11.810	3260	3272	3289	rBV	388997	630220	81.68%	9.140%
23	12.193	3376	3391	3407	rBV	251370	420742	54.53%	6.102%

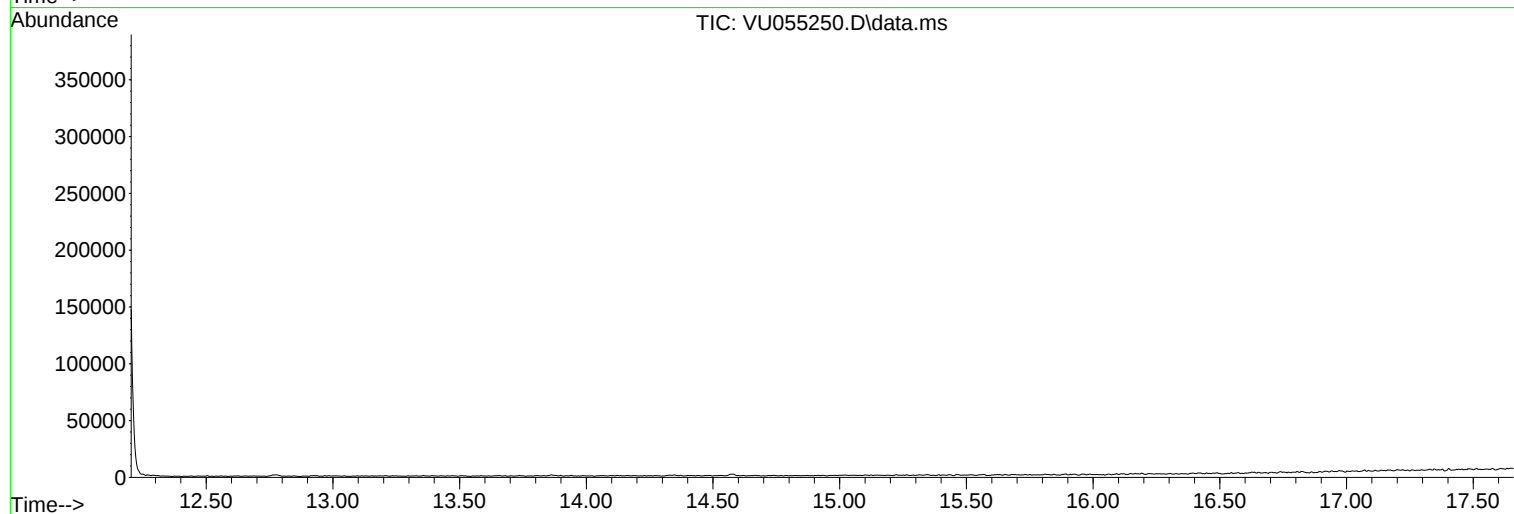
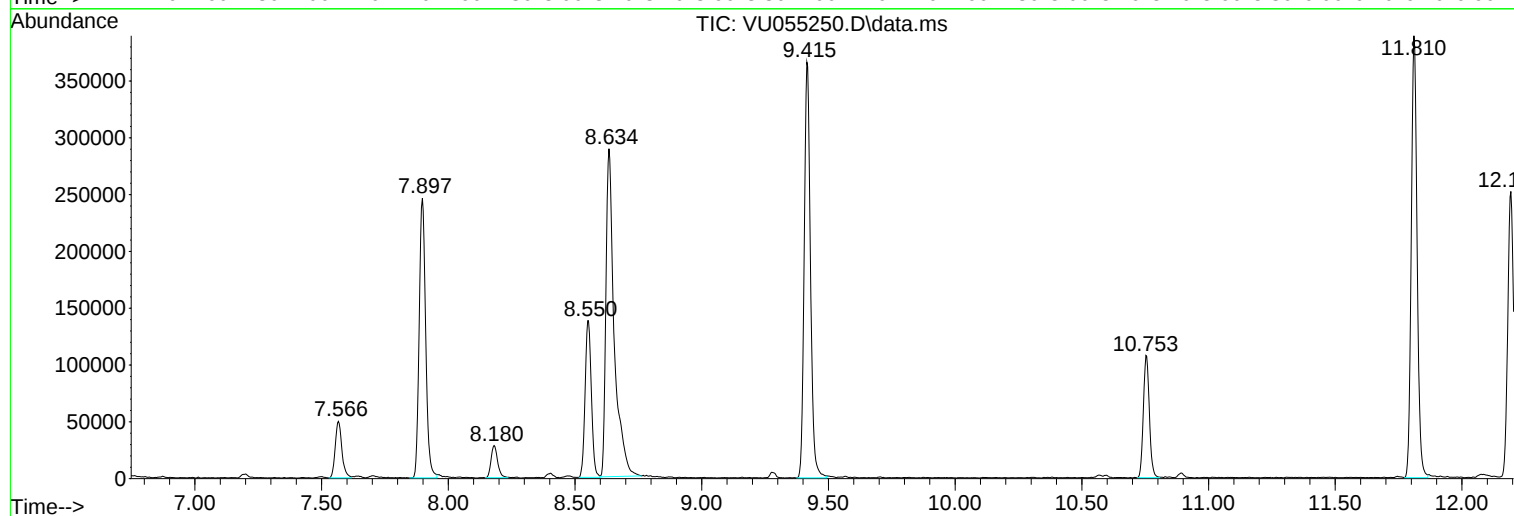
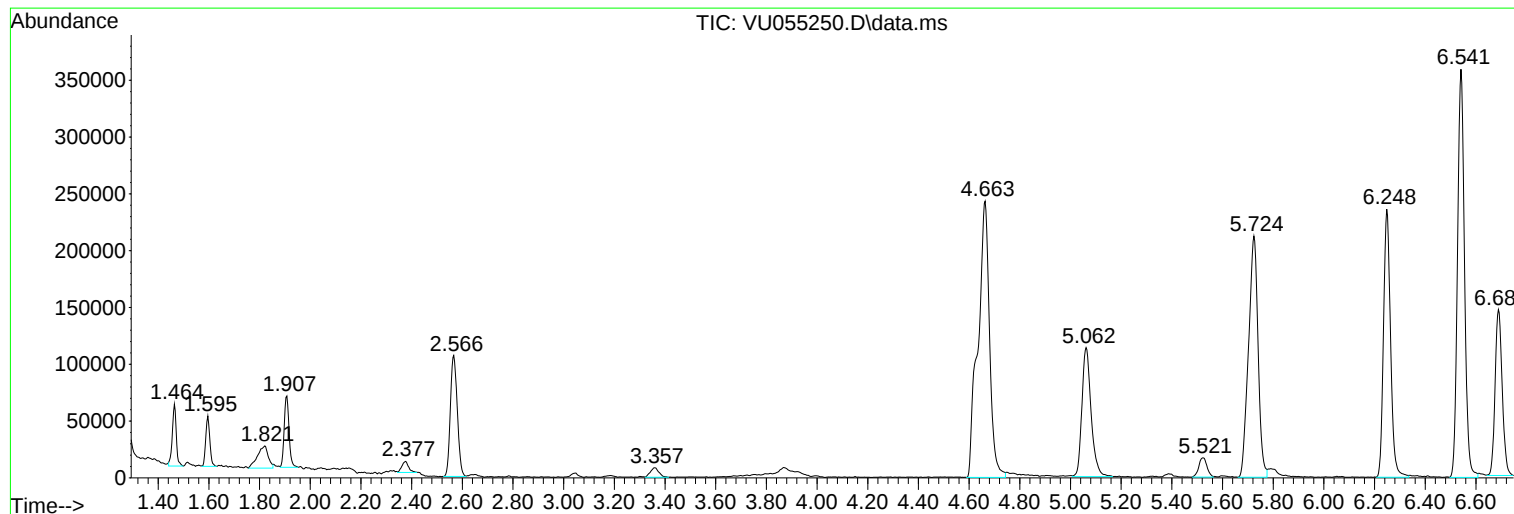
Sum of corrected areas: 6895506

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR090123WMA.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 :
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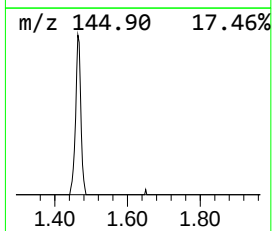
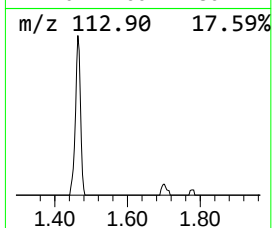
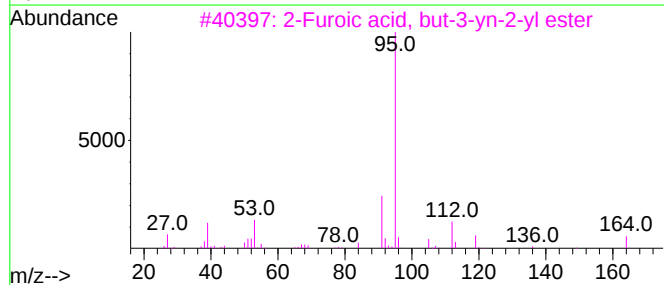
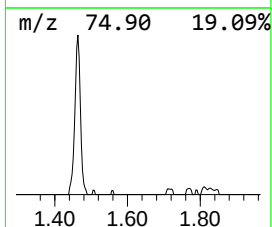
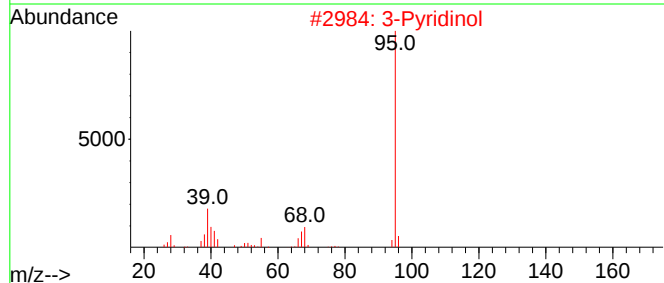
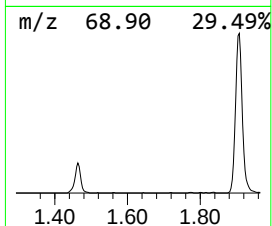
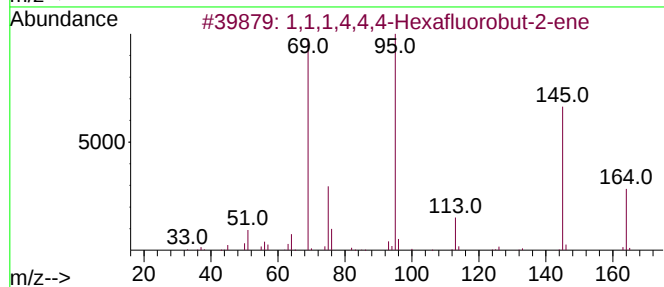
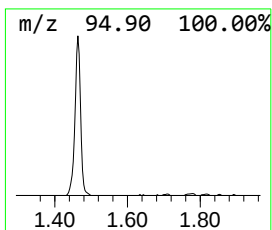
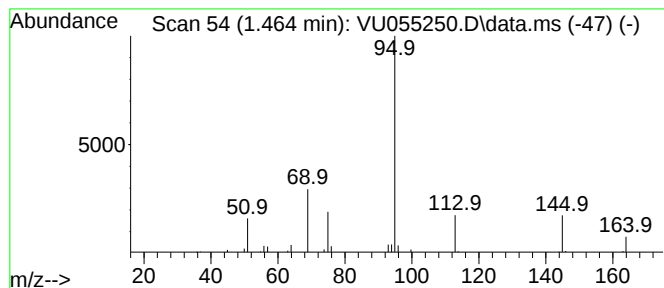
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR090123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.464	0.65 ug/L	58933	1,4-Difluorobenzene	6.248

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,1,4,4,4-Hexafluorobut-2-ene	164	C4H2F6	1010394-40-0	22		
2	3-Pyridinol	95	C5H5NO	000109-00-2	7		
3	2-Furoic acid, but-3-yn-2-yl ester	164	C9H8O3	1000299-23-2	7		
4	3-Pyridinol	95	C5H5NO	000109-00-2	5		
5	4-Pyridinol	95	C5H5NO	000626-64-2	5		



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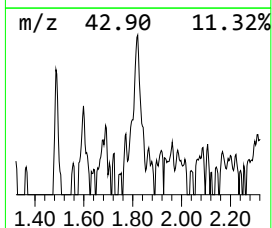
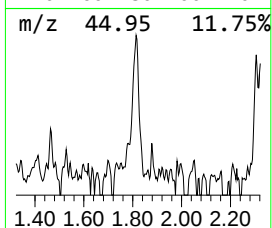
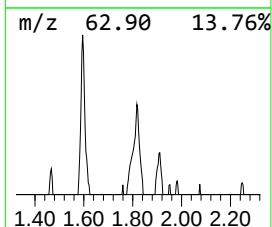
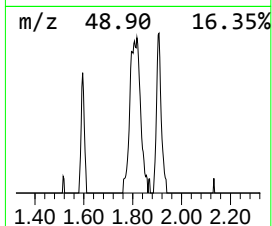
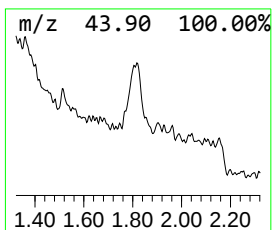
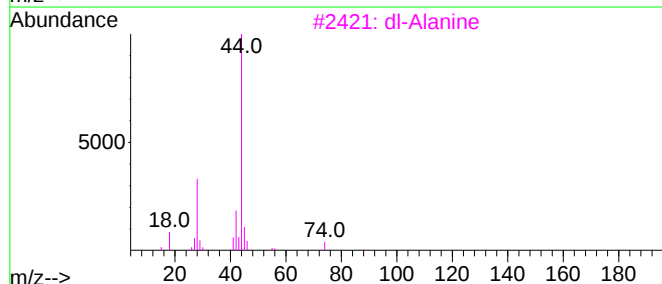
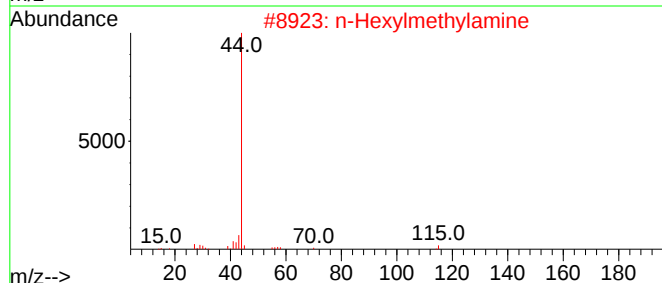
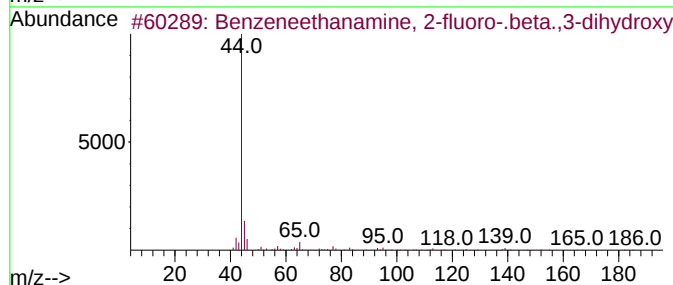
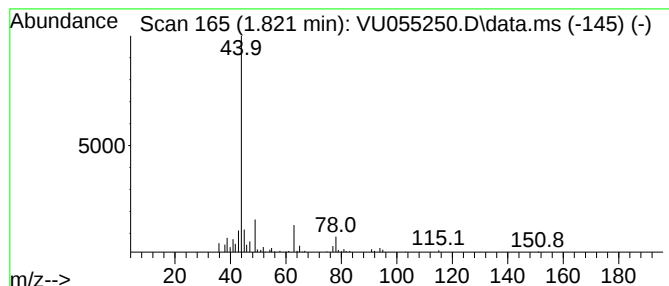
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Benzeneethanamine, 2-fluoro... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.821	0.64 ug/L	58130	1,4-Difluorobenzene	6.248

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzeneethanamine, 2-fluoro-.bet...	185	C9H12FN02	103439-04-9	59
2			n-Hexylmethylamine	115	C7H17N	035161-70-7	49
3			dl-Alanine	89	C3H7NO2	000302-72-7	42
4			Acetic acid, hydroxy[(1-oxo-2-pr...	145	C5H7NO4	006737-24-2	36
5			sec-Butylamine	73	C4H11N	013952-84-6	36



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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	1.464	0.7	ug/L	58933	1	6.248	456529	5.0
Benzeneethanami...	1.821	0.6	ug/L	58130	1	6.248	456529	5.0