

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070824\
 Data File : VU059879.D
 Acq On : 08 Jul 2024 13:31
 Operator : MD/SY
 Sample : P3137-21
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 YDZE3

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\SFAMUTR061724WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU059879.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.329	7	12	18	rBV	91020	94412	13.60%	1.365%
2	1.377	20	27	56	rVV	105433	213896	30.80%	3.092%
3	1.489	57	62	67	rVB	19789	19617	2.82%	0.284%
4	1.592	86	94	108	rVB	62410	83321	12.00%	1.205%
5	1.785	146	154	171	rBV2	135229	218370	31.45%	3.157%
6	1.907	186	192	210	rVB	49215	65735	9.47%	0.950%
7	2.460	354	364	380	rVB2	38852	69017	9.94%	0.998%
8	2.557	383	394	409	rVB	89127	149592	21.54%	2.163%
9	2.653	409	424	444	rBV2	6154	20689	2.98%	0.299%
10	2.785	453	465	477	rBV	42418	75951	10.94%	1.098%
11	3.039	535	544	554	rVB4	7740	13307	1.92%	0.192%
12	3.229	584	603	635	rBV4	33807	193384	27.85%	2.796%
13	3.988	815	839	856	rBV5	11066	37943	5.46%	0.549%
14	4.637	1025	1041	1084	rBV	74108	276545	39.82%	3.998%
15	4.849	1093	1107	1145	rVB3	15090	70300	10.12%	1.016%
16	5.055	1157	1171	1203	rVB2	113133	263262	37.91%	3.806%
17	5.717	1357	1377	1404	rBV2	194217	528354	76.08%	7.639%
18	5.856	1404	1420	1446	rBV4	30586	108961	15.69%	1.575%
19	6.242	1528	1540	1563	rBV	194295	375872	54.13%	5.434%
20	6.640	1654	1664	1666	rBV4	5783	7786	1.12%	0.113%
21	6.685	1666	1678	1696	rVB2	122872	243904	35.12%	3.526%
22	7.052	1768	1792	1794	rBV7	7126	24013	3.46%	0.347%
23	7.161	1818	1826	1836	rVV3	4501	8173	1.18%	0.118%
24	7.216	1836	1843	1856	rVB10	3451	7284	1.05%	0.105%
25	7.438	1901	1912	1922	rVB6	4079	7417	1.07%	0.107%
26	7.563	1938	1951	1968	rBV	54025	110432	15.90%	1.597%
27	7.859	2028	2043	2045	rBV2	45769	64325	9.26%	0.930%
28	7.891	2046	2053	2072	rVV	238822	425535	61.28%	6.152%
29	7.968	2073	2077	2086	rVV2	5077	6985	1.01%	0.101%
30	8.177	2132	2142	2157	rBV3	35586	61856	8.91%	0.894%
31	8.476	2222	2235	2256	rBV3	20093	45925	6.61%	0.664%
32	8.630	2269	2283	2323	rBV	355743	694446	100.00%	10.040%
33	8.788	2327	2332	2344	rVB8	3638	7098	1.02%	0.103%
34	9.267	2467	2481	2492	rBV2	6064	11419	1.64%	0.165%
35	9.335	2492	2502	2514	rVV2	17201	28514	4.11%	0.412%
36	9.412	2514	2526	2553	rBV	291319	498305	71.76%	7.204%

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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_U\Method\SFAMUTR061724WMA.M
 Title : TRACE VOA SFAM1.0

37	9.573	2566	2576	2596	rVB4	9563	19392	2.79%	0.280%
38	9.701	2601	2616	2628	rBV4	17915	36410	5.24%	0.526%
39	10.052	2716	2725	2733	rVB9	4407	8267	1.19%	0.120%
40	10.097	2733	2739	2752	rVB3	6620	10216	1.47%	0.148%
41	10.486	2857	2860	2872	rVB8	4405	7017	1.01%	0.101%
42	10.640	2897	2908	2917	rBV6	11580	18858	2.72%	0.273%
43	10.749	2931	2942	2957	rBV	123344	204417	29.44%	2.955%
44	10.888	2967	2985	2996	rBV	78317	132120	19.03%	1.910%
45	11.228	3080	3091	3103	rVB9	5900	9966	1.44%	0.144%
46	11.470	3156	3166	3176	rVB3	8236	14624	2.11%	0.211%
47	11.531	3176	3185	3198	rBV8	7897	14438	2.08%	0.209%
48	11.634	3210	3217	3226	rVB9	4471	7111	1.02%	0.103%
49	11.807	3256	3271	3292	rVV	296842	490678	70.66%	7.094%
50	11.897	3292	3299	3311	rVV	4952	10361	1.49%	0.150%
51	12.058	3340	3349	3366	rBV5	16869	41469	5.97%	0.600%
52	12.151	3369	3378	3379	rVV2	8979	11890	1.71%	0.172%
53	12.190	3379	3390	3410	rVB	250970	429105	61.79%	6.204%
54	12.470	3472	3477	3490	rVB8	3791	7519	1.08%	0.109%
55	12.762	3562	3568	3577	rBV2	5159	7348	1.06%	0.106%
56	13.019	3641	3648	3660	rVB8	5802	11546	1.66%	0.167%
57	13.412	3763	3770	3776	rBV8	4034	6966	1.00%	0.101%
58	13.453	3776	3783	3791	rVB7	4316	6977	1.00%	0.101%
59	13.675	3843	3852	3862	rVV5	8035	13994	2.02%	0.202%
60	13.730	3865	3869	3877	rVB6	6107	8053	1.16%	0.116%
61	13.842	3894	3904	3908	rBV9	5030	7932	1.14%	0.115%
62	14.100	3974	3984	3996	rVB4	7439	15046	2.17%	0.218%
63	14.283	4033	4041	4050	rBV4	4187	7954	1.15%	0.115%
64	14.344	4054	4060	4070	rVB7	7339	10723	1.54%	0.155%
65	14.576	4122	4132	4138	rBV2	6503	9285	1.34%	0.134%
66	15.023	4262	4271	4283	rVB2	5311	11133	1.60%	0.161%
67	15.228	4329	4335	4343	rVB7	4689	8135	1.17%	0.118%
68	15.347	4366	4372	4379	rVV5	8624	14885	2.14%	0.215%
69	15.402	4381	4389	4401	rVB5	11788	27897	4.02%	0.403%
70	15.563	4432	4439	4449	rVB5	7739	12695	1.83%	0.184%
71	15.685	4467	4477	4492	rBV7	12548	30725	4.42%	0.444%
72	15.820	4511	4519	4526	rBV7	4807	7799	1.12%	0.113%
73	15.916	4541	4549	4551	rBV7	5769	7743	1.11%	0.112%
74	16.003	4568	4576	4591	rVB5	11827	21897	3.15%	0.317%
75	16.177	4624	4630	4640	rBV5	7556	15077	2.17%	0.218%
76	16.418	4700	4705	4714	rVB9	6306	8710	1.25%	0.126%

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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 >
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Title : TRACE VOA SFAM1.0

77	16.624	4762	4769	4777	rBV9	7454	13317	1.92%	0.193%
78	17.257	4960	4966	4973	rVB9	8405	12185	1.75%	0.176%
79	17.350	4992	4995	5008	rVB9	9799	13087	1.88%	0.189%

Sum of corrected areas: 6916912

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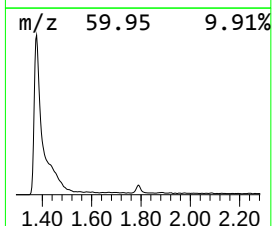
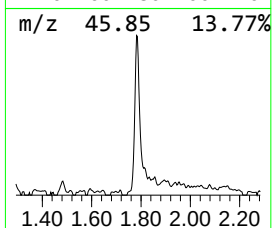
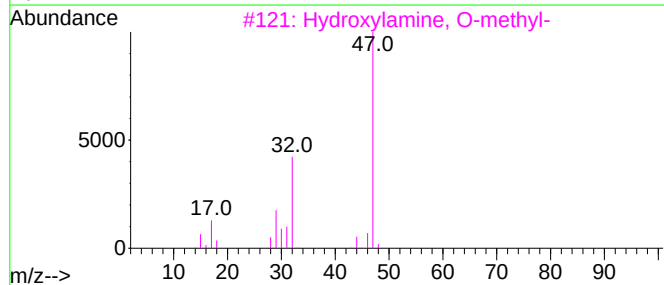
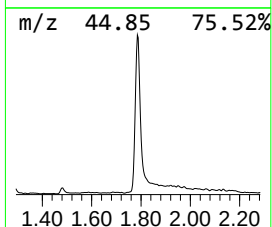
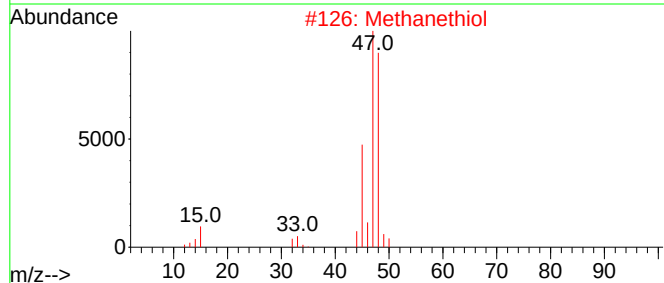
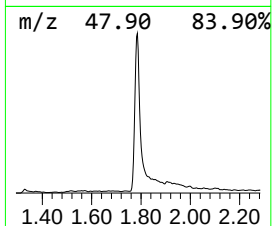
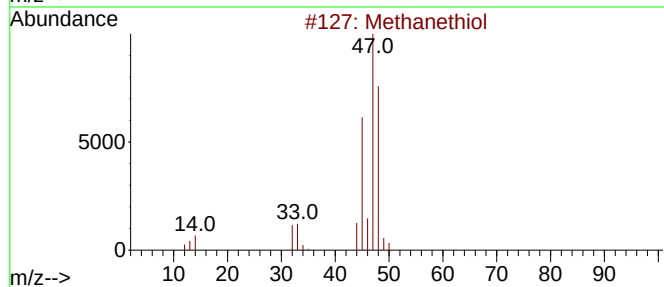
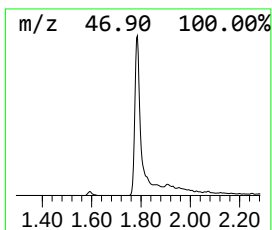
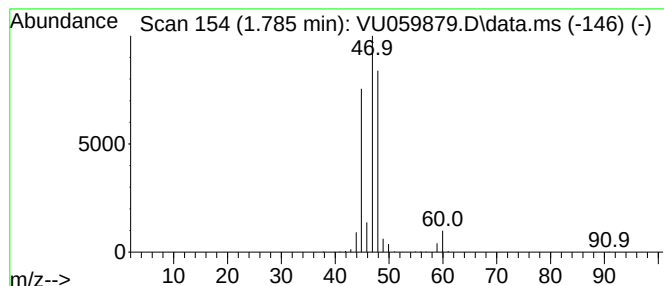
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Methanethiol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.785	2.90 ug/L	218370	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanethiol	48	CH4S	000074-93-1	86
2			Methanethiol	48	CH4S	000074-93-1	72
3			Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
4			Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
5			Methane, nitroso-	45	CH3NO	000865-40-7	5



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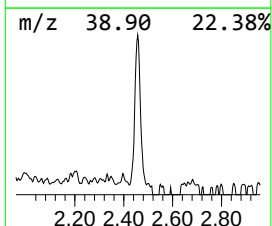
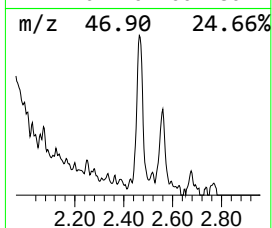
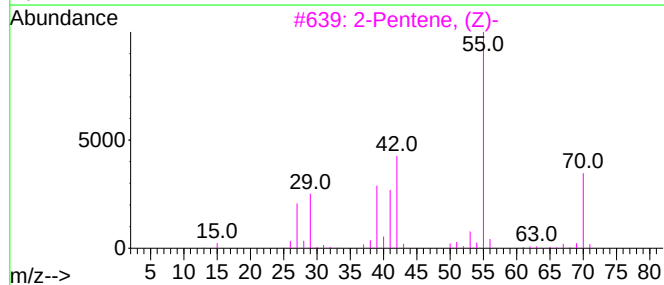
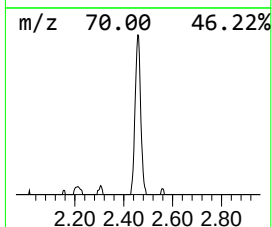
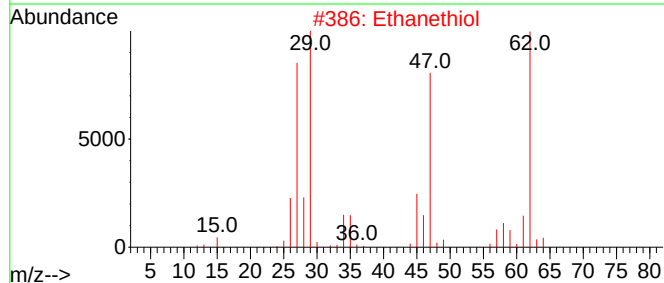
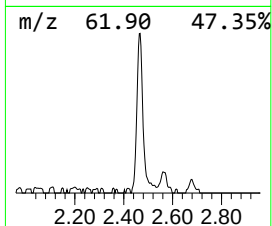
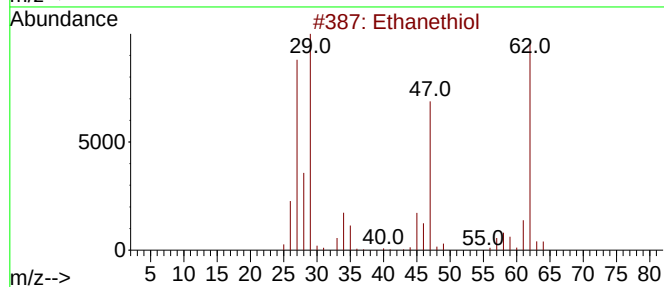
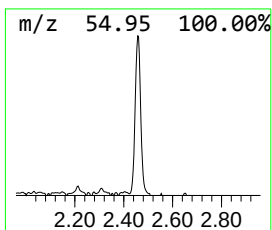
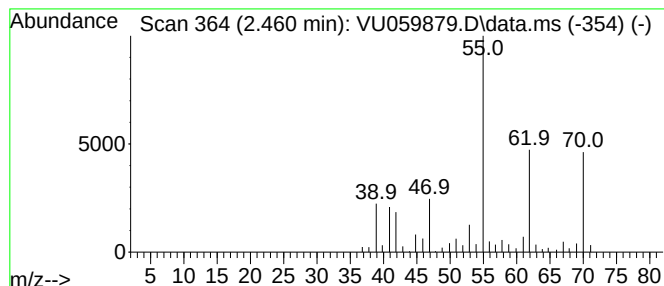
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Ethanethiol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.460	0.92 ug/L	69017	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanethiol	62	C2H6S	000075-08-1	53
2			Ethanethiol	62	C2H6S	000075-08-1	42
3			2-Pentene, (Z)-	70	C5H10	000627-20-3	11
4			2-Pentene, (E)-	70	C5H10	000646-04-8	11
5			2-Pentene, (Z)-	70	C5H10	000627-20-3	11



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Instrument :
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ClientSampleId :
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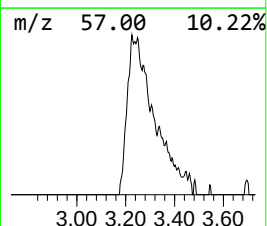
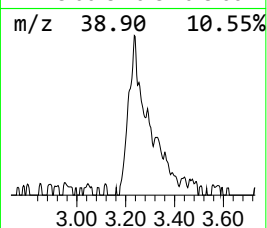
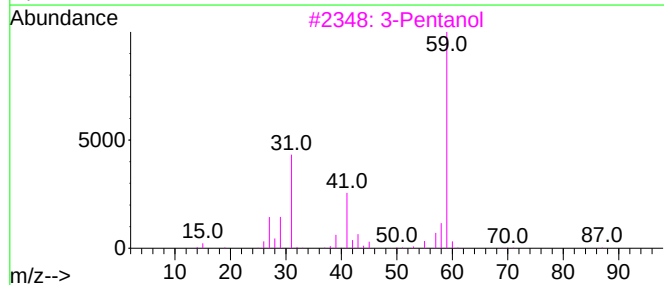
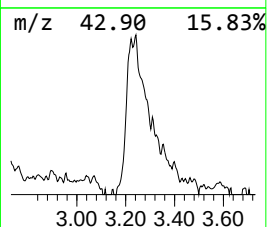
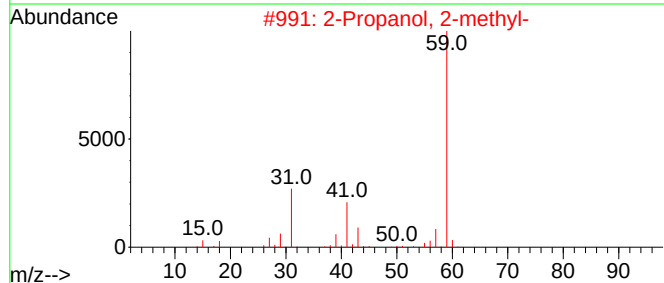
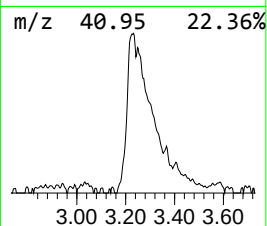
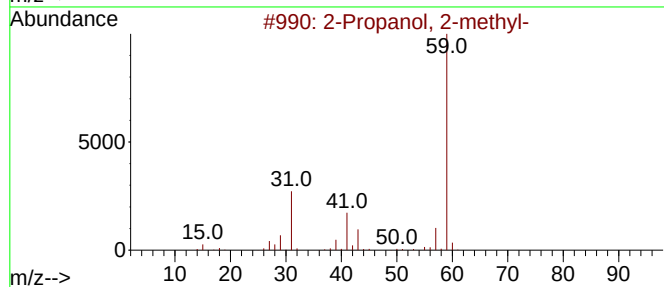
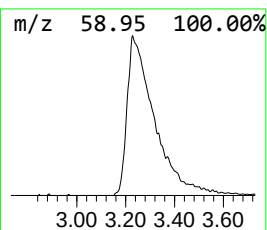
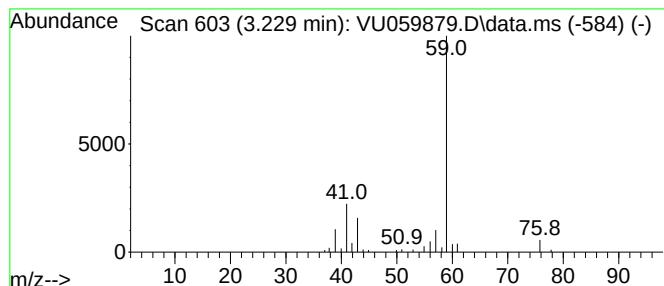
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 2-Propanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.229	2.57 ug/L	193384	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	56
2	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	56
3	3-Pentanol			88	C5H12O	000584-02-1	50
4	Acetic acid, cyano-, 1,1-dimethy...			141	C7H11NO2	001116-98-9	45
5	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	40



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MSVOA_U
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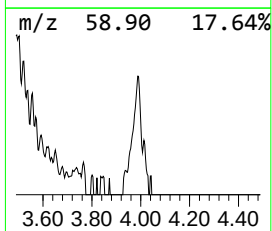
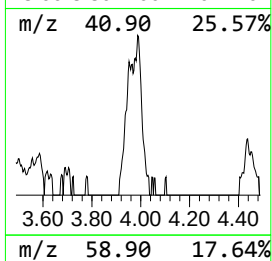
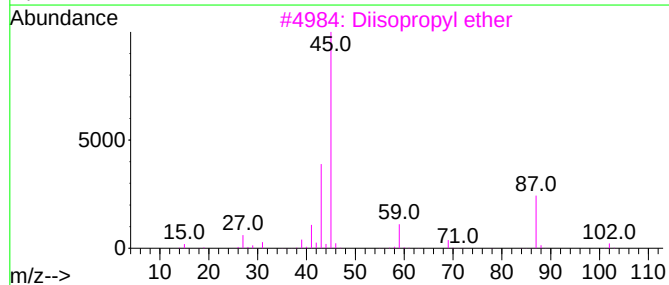
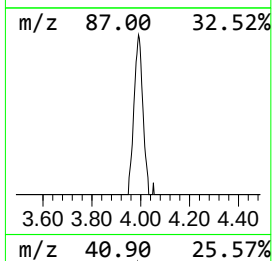
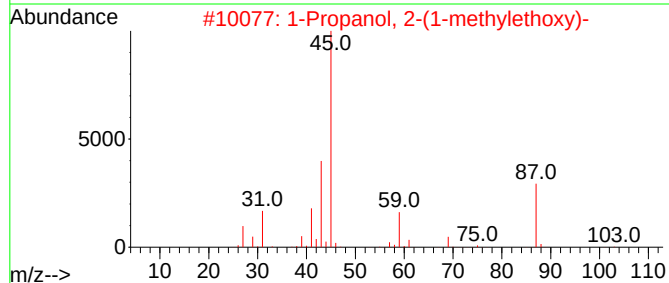
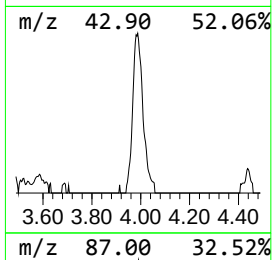
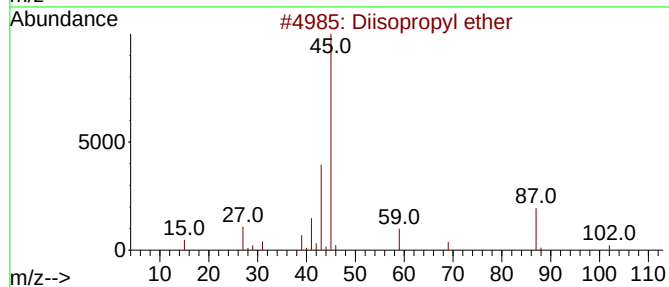
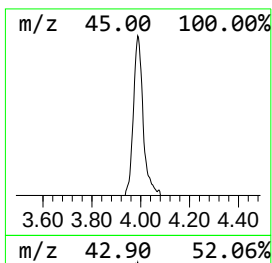
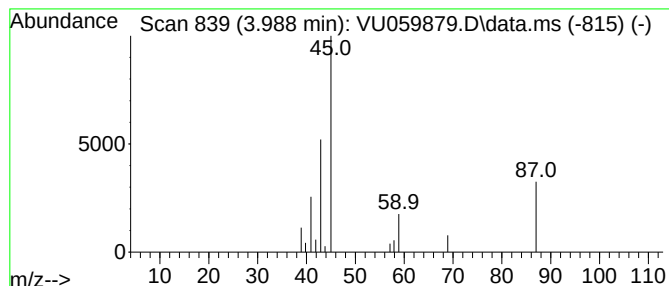
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Diisopropyl ether Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.988	0.50 ug/L	37943	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diisopropyl ether	102	C6H14O	000108-20-3	78
2			1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	74
3			Diisopropyl ether	102	C6H14O	000108-20-3	64
4			Diisopropyl ether	102	C6H14O	000108-20-3	64
5			1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070824\
Data File : VU059879.D
Acq On : 08 Jul 2024 13:31
Operator : MD/SY
Sample : P3137-21
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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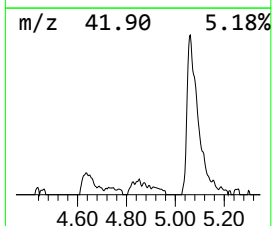
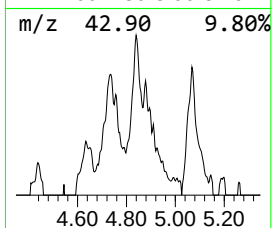
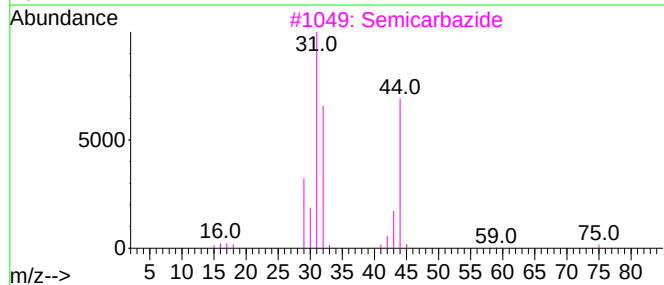
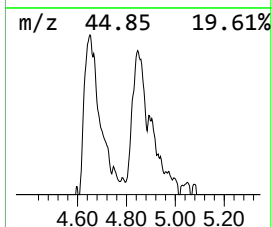
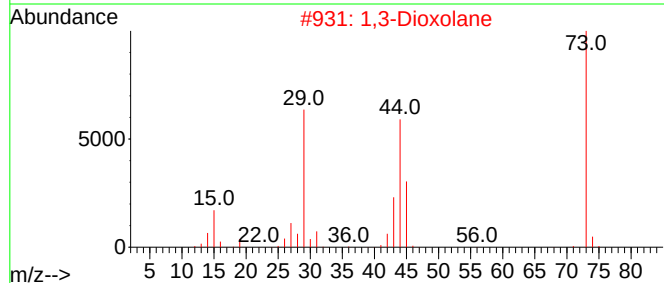
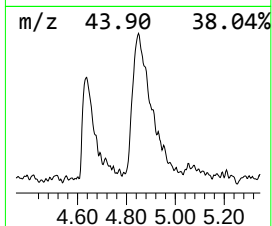
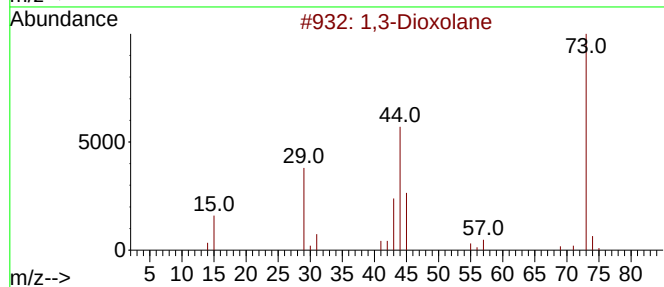
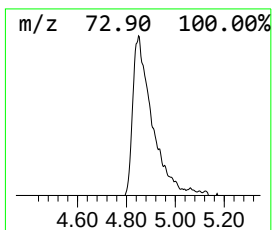
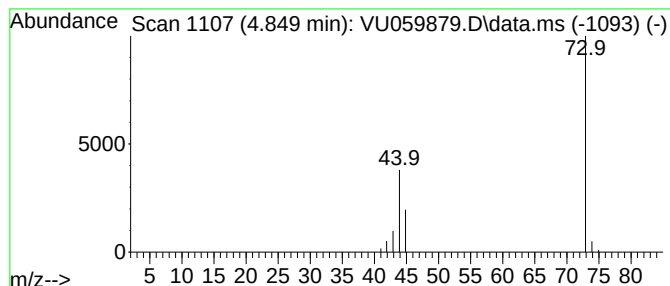
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 1,3-Dioxolane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.849	0.94 ug/L	70300	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane			74	C3H6O2	000646-06-0	83
2	1,3-Dioxolane			74	C3H6O2	000646-06-0	9
3	Semicarbazide			75	CH5N3O	004426-72-6	7
4	N-Ethylformamide			73	C3H7NO	000627-45-2	7
5	1,3-Dioxolane			74	C3H6O2	000646-06-0	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070824\
Data File : VU059879.D
Acq On : 08 Jul 2024 13:31
Operator : MD/SY
Sample : P3137-21
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YDZE3

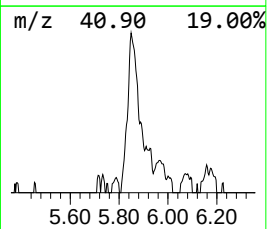
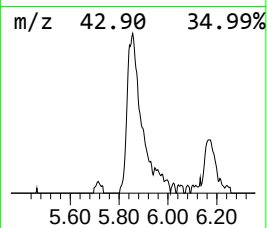
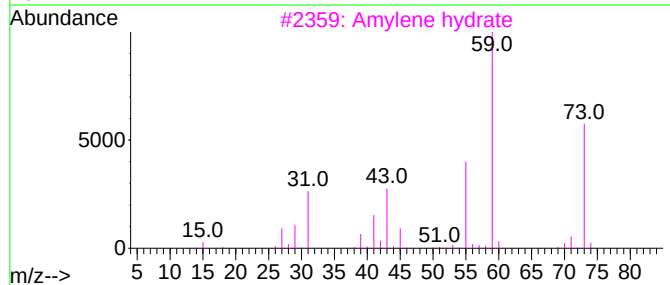
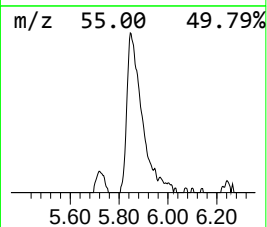
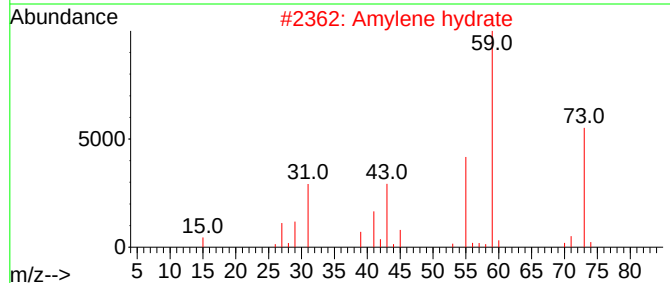
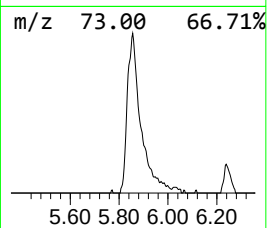
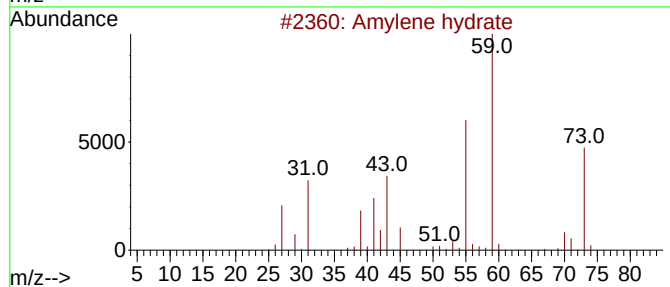
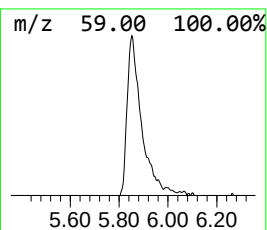
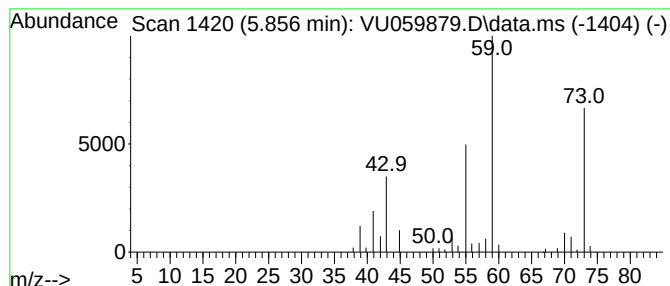
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 Amylene hydrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.856	1.45 ug/L	108961	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	78
2			Amylene hydrate	88	C5H12O	000075-85-4	78
3			Amylene hydrate	88	C5H12O	000075-85-4	78
4			Amylene hydrate	88	C5H12O	000075-85-4	56
5			Amylene hydrate	88	C5H12O	000075-85-4	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070824\
Data File : VU059879.D
Acq On : 08 Jul 2024 13:31
Operator : MD/SY
Sample : P3137-21
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
YDZE3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methanethiol	1.785	2.9	ug/L	218370	1	6.245	375872	5.0
Ethanethiol	2.460	0.9	ug/L	69017	1	6.245	375872	5.0
2-Propanol, 2-m...	3.229	2.6	ug/L	193384	1	6.245	375872	5.0
Diisopropyl ether	3.988	0.5	ug/L	37943	1	6.245	375872	5.0
1,3-Dioxolane	4.849	0.9	ug/L	70300	1	6.245	375872	5.0
Amylene hydrate	5.856	1.5	ug/L	108961	1	6.245	375872	5.0