

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU090123\
 Data File : VU055074.D
 Acq On : 02 Sep 2023 05:09
 Operator : MD/SY
 Sample : 04250-11
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH4E8

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: VU055074.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.354	14	20	35	rBV3	12442	18908	2.85%	0.268%
2	1.483	52	60	66	rBV	86473	145403	21.94%	2.061%
3	1.595	90	95	107	rVB	67816	84466	12.74%	1.197%
4	1.911	186	193	208	rVB	76448	103451	15.61%	1.466%
5	2.563	385	396	409	rBV	128207	213565	32.22%	3.027%
6	2.637	409	419	444	rVV	41876	98409	14.85%	1.395%
7	2.956	509	518	535	rBV	14609	27328	4.12%	0.387%
8	3.039	535	544	557	rVB	16042	29240	4.41%	0.414%
9	3.351	632	641	652	rBV6	4485	9711	1.47%	0.138%
10	4.631	1028	1039	1064	rBV2	79216	268807	40.55%	3.809%
11	4.820	1089	1098	1114	rVB5	4492	11344	1.71%	0.161%
12	5.058	1156	1172	1198	rBV	144299	335343	50.59%	4.752%
13	5.721	1359	1378	1402	rBV3	255695	662839	100.00%	9.394%
14	6.245	1525	1541	1570	rBV	232957	460319	69.45%	6.524%
15	6.541	1621	1633	1647	rBV2	44410	90088	13.59%	1.277%
16	6.689	1665	1679	1702	rBV	160347	321187	48.46%	4.552%
17	7.563	1940	1951	1971	rBV2	54664	101336	15.29%	1.436%
18	7.795	2012	2023	2042	rBV2	13473	27201	4.10%	0.385%
19	7.894	2042	2054	2068	rBV	308773	549098	82.84%	7.782%
20	7.968	2068	2077	2091	rVB	63915	115618	17.44%	1.639%
21	8.177	2130	2142	2160	rBV2	31917	58150	8.77%	0.824%
22	8.550	2249	2258	2261	rBV6	6323	8760	1.32%	0.124%
23	8.634	2273	2284	2321	rBV4	252907	584157	88.13%	8.279%
24	8.788	2323	2332	2338	rVV3	31413	54629	8.24%	0.774%
25	8.833	2338	2346	2377	rVB2	106794	205040	30.93%	2.906%
26	9.415	2515	2527	2550	rBV	348157	605987	91.42%	8.588%
27	9.569	2565	2575	2589	rVB2	13263	22482	3.39%	0.319%
28	9.692	2600	2613	2627	rVB2	33547	59309	8.95%	0.841%
29	10.113	2725	2744	2762	rBV7	50848	111147	16.77%	1.575%
30	10.238	2769	2783	2798	rBV3	7799	14693	2.22%	0.208%
31	10.348	2802	2817	2828	rBV7	7067	17930	2.71%	0.254%
32	10.753	2929	2943	2958	rBV	112777	186283	28.10%	2.640%
33	11.473	3156	3167	3184	rBV5	7452	17896	2.70%	0.254%
34	11.692	3224	3235	3247	rBV6	10656	20316	3.06%	0.288%
35	11.811	3259	3272	3290	rBV	398395	653816	98.64%	9.266%
36	11.907	3290	3302	3311	rVB	4959	9915	1.50%	0.141%

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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

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Title : TRACE VOA SFAM1.0

37	12.058	3337	3349	3367	rBV3	73266	152672	23.03%	2.164%
38	12.190	3378	3390	3405	rBV	301371	506487	76.41%	7.178%
39	12.775	3564	3572	3581	rBV7	7135	11816	1.78%	0.167%
40	12.888	3599	3607	3621	rBV5	14804	24682	3.72%	0.350%
41	13.209	3699	3707	3716	rBV8	4897	7925	1.20%	0.112%
42	13.843	3894	3904	3916	rBV4	13679	23639	3.57%	0.335%
43	13.962	3932	3941	3948	rBV9	4605	7031	1.06%	0.100%
44	14.093	3968	3982	3990	rBV5	3745	7649	1.15%	0.108%
45	14.331	4044	4056	4065	rBV5	5423	10196	1.54%	0.144%

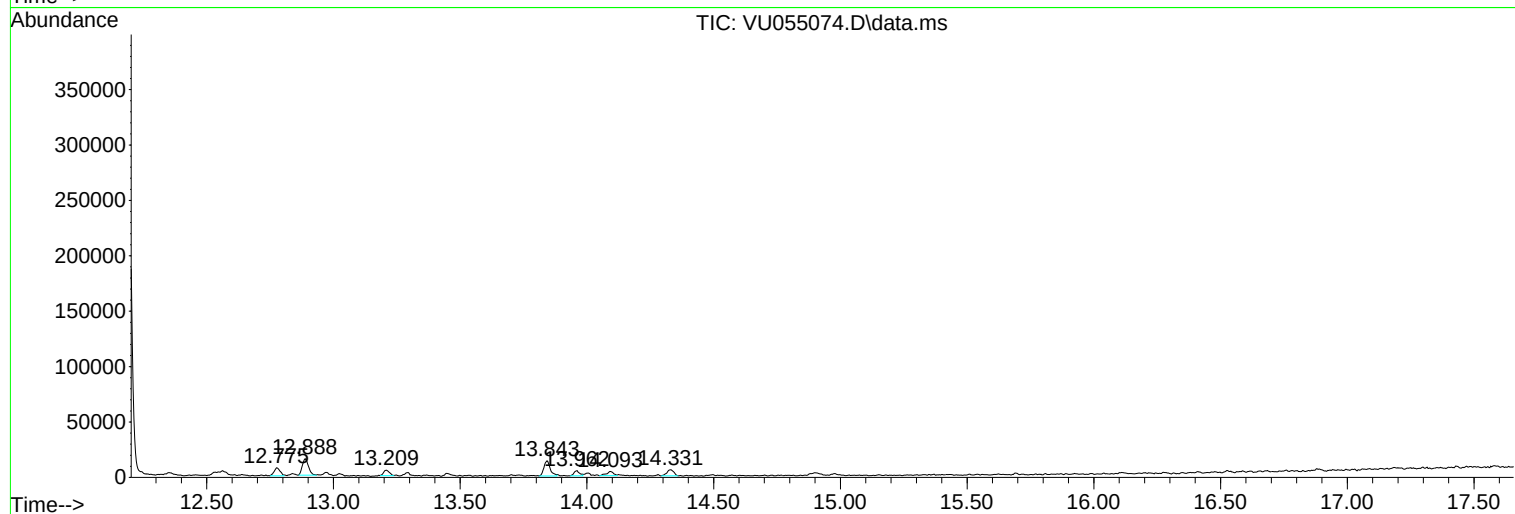
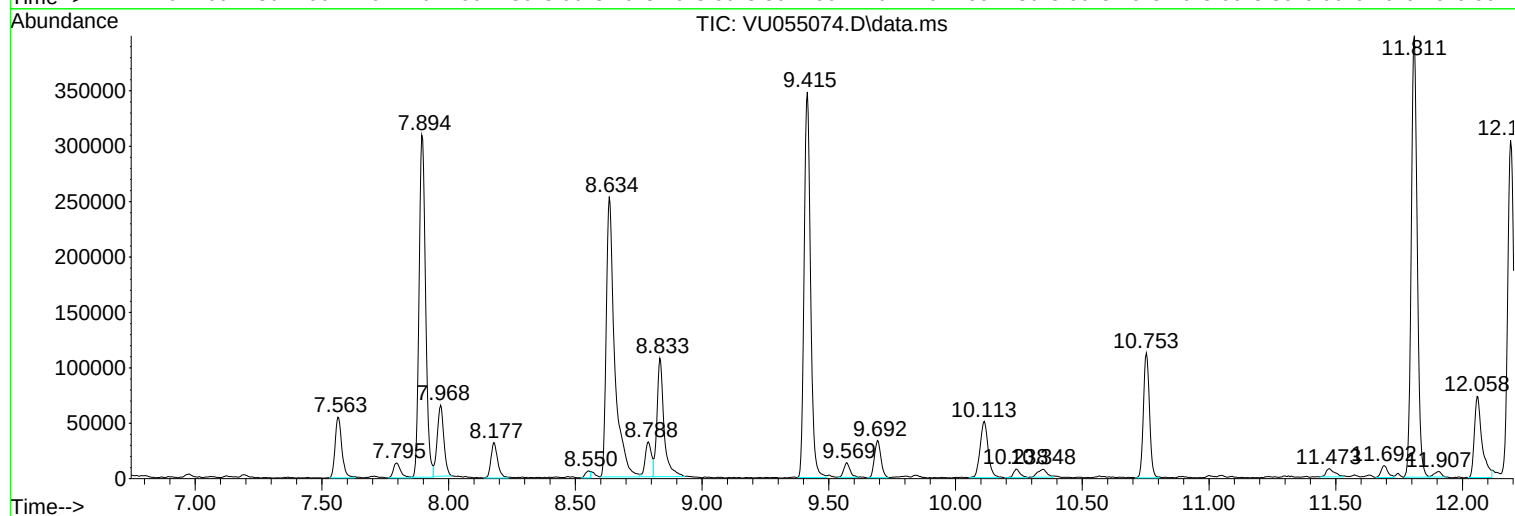
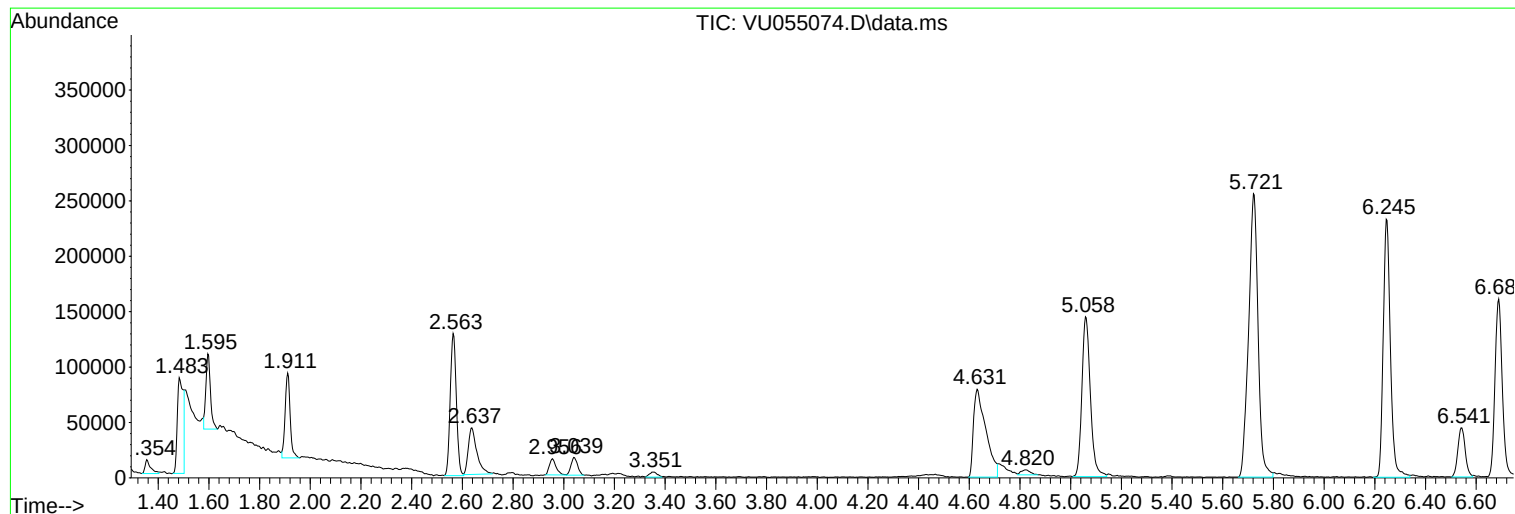
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR090123WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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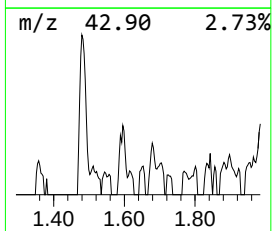
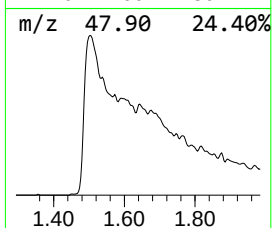
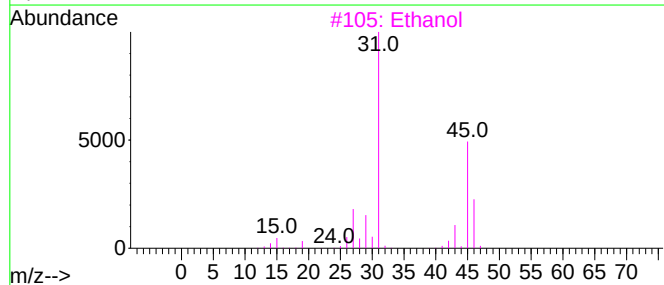
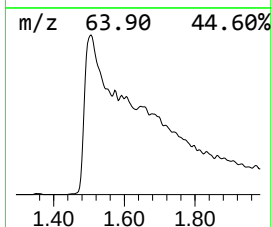
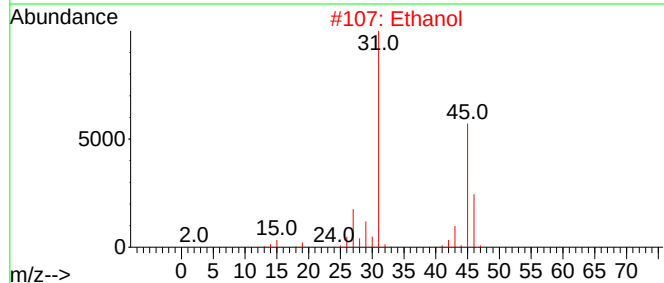
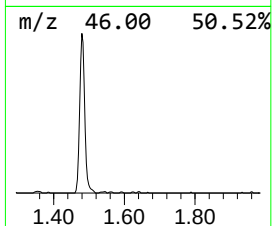
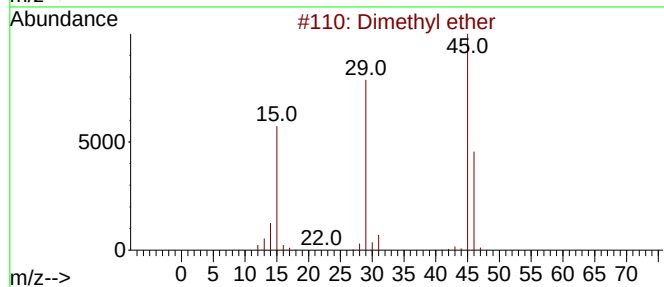
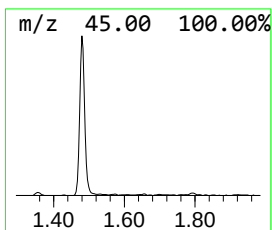
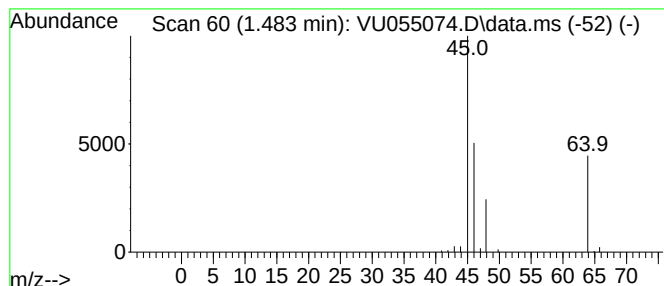
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR090123WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
1.483	1.58 ug/L	145403	1,4-Difluorobenzene	6.248

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	16
2			Ethanol	46	C2H6O	000064-17-5	9
3			Ethanol	46	C2H6O	000064-17-5	9
4			Dimethyl ether	46	C2H6O	000115-10-6	9
5			Dimethyl ether	46	C2H6O	000115-10-6	7



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ALS Vial : 44 Sample Multiplier: 1

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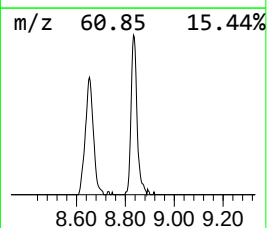
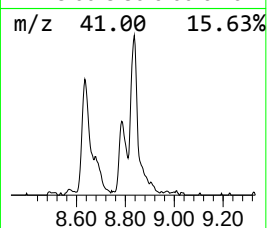
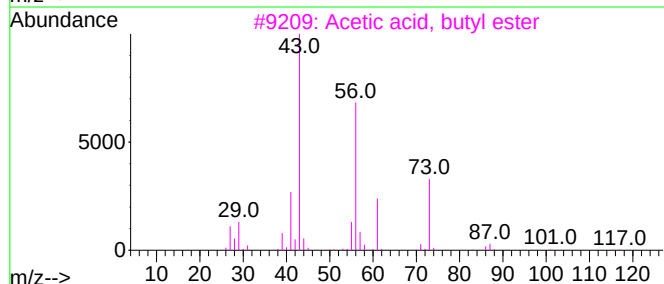
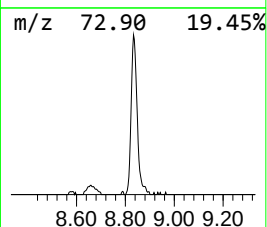
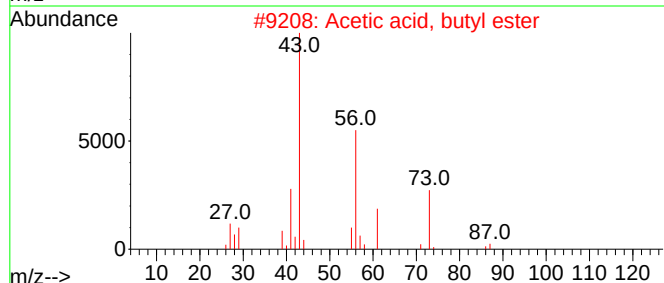
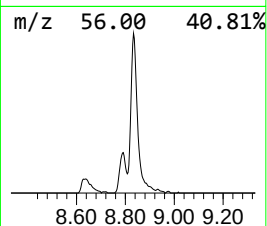
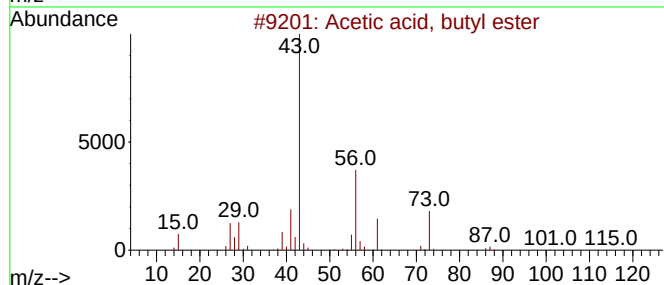
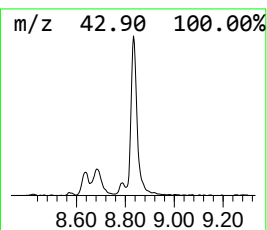
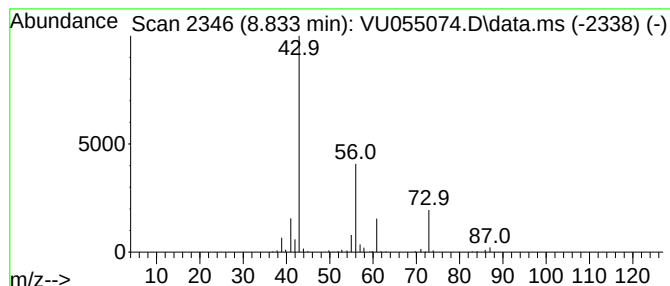
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR090123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Acetic acid, butyl ester Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.833	1.69 ug/L	205040	Chlorobenzene-d5	9.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester		116	C6H12O2	000123-86-4	83	
2	Acetic acid, butyl ester		116	C6H12O2	000123-86-4	56	
3	Acetic acid, butyl ester		116	C6H12O2	000123-86-4	50	
4	Acetic acid, butyl ester		116	C6H12O2	000123-86-4	25	
5	1,4-Butanediol, diacetate		174	C8H14O4	000628-67-1	12	



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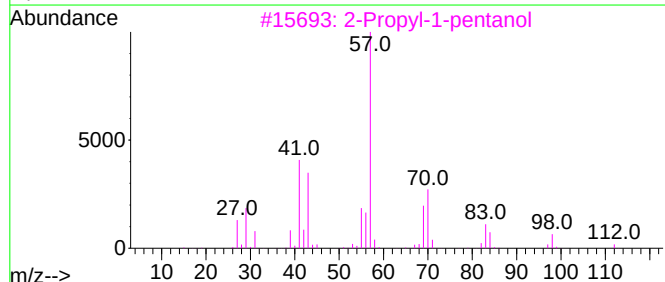
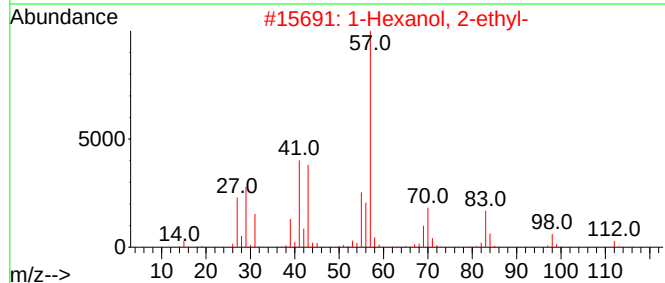
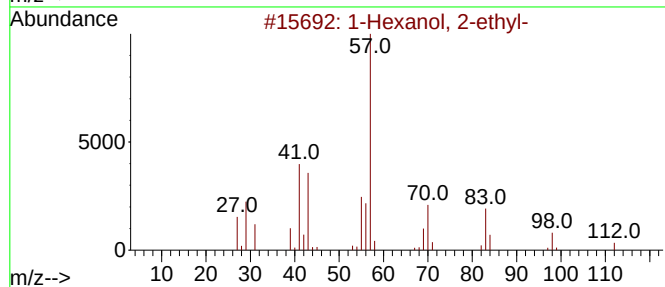
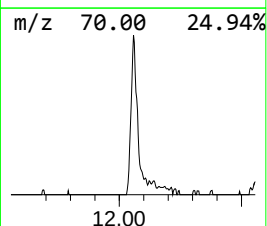
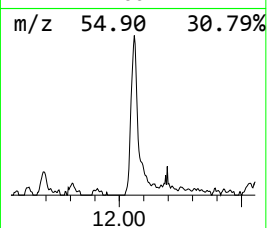
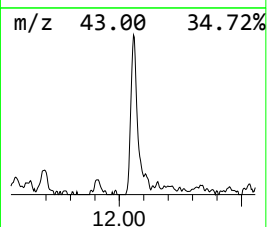
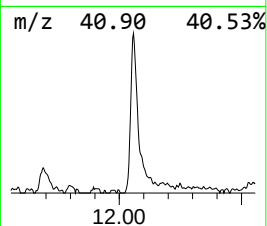
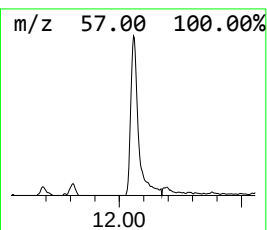
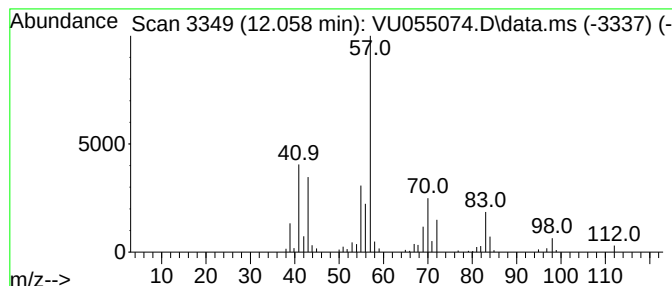
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.058	1.17 ug/L	152672	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
3			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	56
5			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53



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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	1.483	1.6	ug/L	145403	1	6.248	460319	5.0
Acetic acid, bu...	8.833	1.7	ug/L	205040	2	9.415	605987	5.0
1-Hexanol, 2-et...	12.058	1.2	ug/L	152672	3	11.810	653816	5.0