

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU090523\
 Data File : VU055099.D
 Acq On : 05 Sep 2023 17:13
 Operator : MD/SY
 Sample : 04250-11
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 19 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: VU055099.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	33	rBV3	10125	15040	2.31%	0.221%
2	1.480	52	59	66	rBV	68484	67470	10.37%	0.990%
3	1.515	66	70	84	rVV2	4728	8238	1.27%	0.121%
4	1.592	86	94	106	rVV	52580	64888	9.97%	0.952%
5	1.907	184	192	202	rBV	63588	81246	12.49%	1.193%
6	2.560	383	395	407	rBV	124457	201298	30.94%	2.955%
7	2.628	407	416	440	rVB	64542	120078	18.46%	1.763%
8	2.792	454	467	476	rBV7	3679	8135	1.25%	0.119%
9	2.952	508	517	530	rBV2	15988	30067	4.62%	0.441%
10	3.039	535	544	556	rVB3	17961	31471	4.84%	0.462%
11	3.358	630	643	653	rBV4	4670	9199	1.41%	0.135%
12	4.624	1028	1037	1061	rBV	89753	233667	35.92%	3.430%
13	4.817	1091	1097	1107	rBV3	4090	7763	1.19%	0.114%
14	5.062	1156	1173	1199	rBV2	138444	322567	49.58%	4.735%
15	5.724	1355	1379	1404	rBV2	244358	629567	96.77%	9.241%
16	6.248	1528	1542	1561	rBV	228713	445643	68.50%	6.541%
17	6.531	1621	1630	1631	rBV4	7262	7329	1.13%	0.108%
18	6.689	1666	1679	1698	rBV2	153659	305016	46.88%	4.477%
19	6.972	1762	1767	1782	rVB7	4205	6993	1.07%	0.103%
20	7.566	1941	1952	1971	rBV3	57431	104322	16.03%	1.531%
21	7.795	2011	2023	2037	rBV3	14229	28397	4.36%	0.417%
22	7.898	2041	2055	2069	rVV	288540	514571	79.09%	7.553%
23	7.968	2069	2077	2097	rVB	62726	115635	17.77%	1.697%
24	8.181	2132	2143	2157	rBV2	35150	61503	9.45%	0.903%
25	8.553	2247	2259	2273	rBV2	7288	17581	2.70%	0.258%
26	8.634	2273	2284	2322	rVV2	275903	610232	93.80%	8.957%
27	8.788	2322	2332	2339	rVV3	63045	104881	16.12%	1.539%
28	8.833	2339	2346	2367	rVB	108531	186694	28.70%	2.740%
29	9.418	2516	2528	2545	rBV	346684	592414	91.06%	8.696%
30	9.573	2565	2576	2587	rBV	14262	22995	3.53%	0.338%
31	9.695	2604	2614	2630	rBV3	33336	58983	9.07%	0.866%
32	10.116	2729	2745	2762	rBV4	51513	111001	17.06%	1.629%
33	10.242	2772	2784	2799	rBV3	9265	17565	2.70%	0.258%
34	10.344	2801	2816	2828	rVV8	8641	21840	3.36%	0.321%
35	10.756	2931	2944	2960	rBV	113541	187676	28.85%	2.755%
36	11.476	3160	3168	3182	rVB4	9827	18255	2.81%	0.268%

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37	11.688	3225	3234	3248	rBV7	12782	22891	3.52%	0.336%
38	11.811	3259	3272	3291	rBV	392329	650601	100.00%	9.550%
39	11.907	3294	3302	3312	rVB8	6262	11707	1.80%	0.172%
40	12.061	3339	3350	3376	rBV2	84591	185190	28.46%	2.718%
41	12.193	3379	3391	3409	rVB	294640	489935	75.30%	7.191%
42	12.348	3433	3439	3455	rVB	3718	7858	1.21%	0.115%
43	12.560	3502	3505	3519	rVB9	5844	9154	1.41%	0.134%
44	12.778	3566	3573	3584	rVB5	8094	13013	2.00%	0.191%
45	12.891	3599	3608	3622	rVB6	20192	33624	5.17%	0.494%
46	13.212	3698	3708	3717	rBV6	5931	10166	1.56%	0.149%
47	13.955	3933	3939	3946	rBV6	5867	8493	1.31%	0.125%

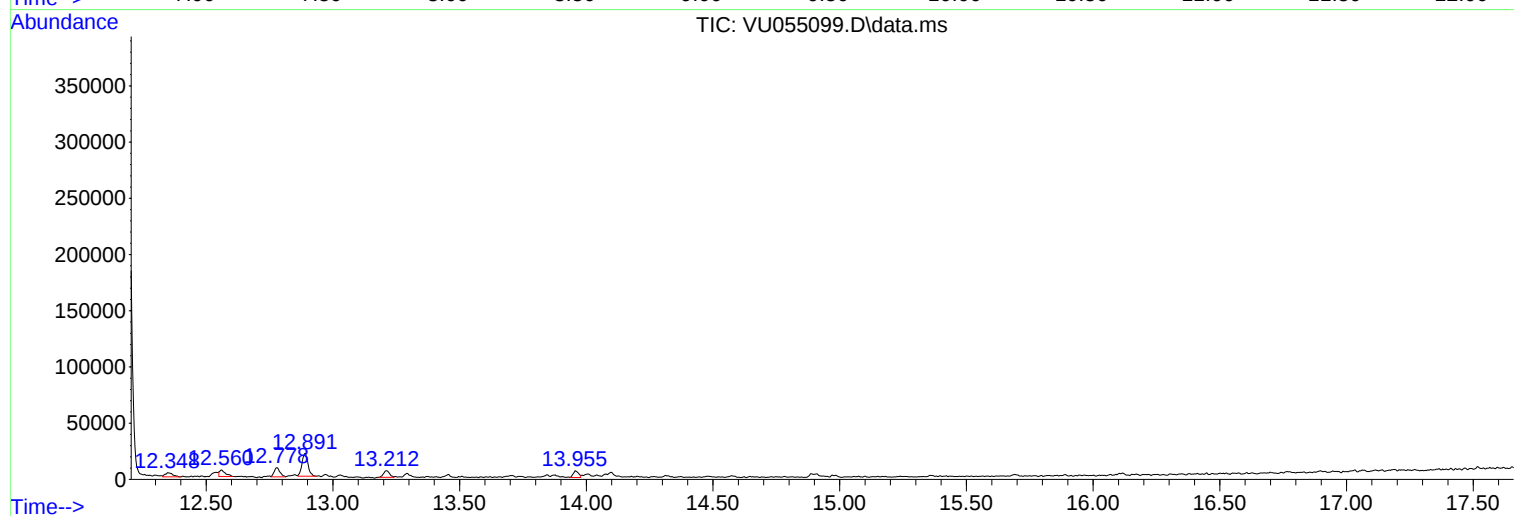
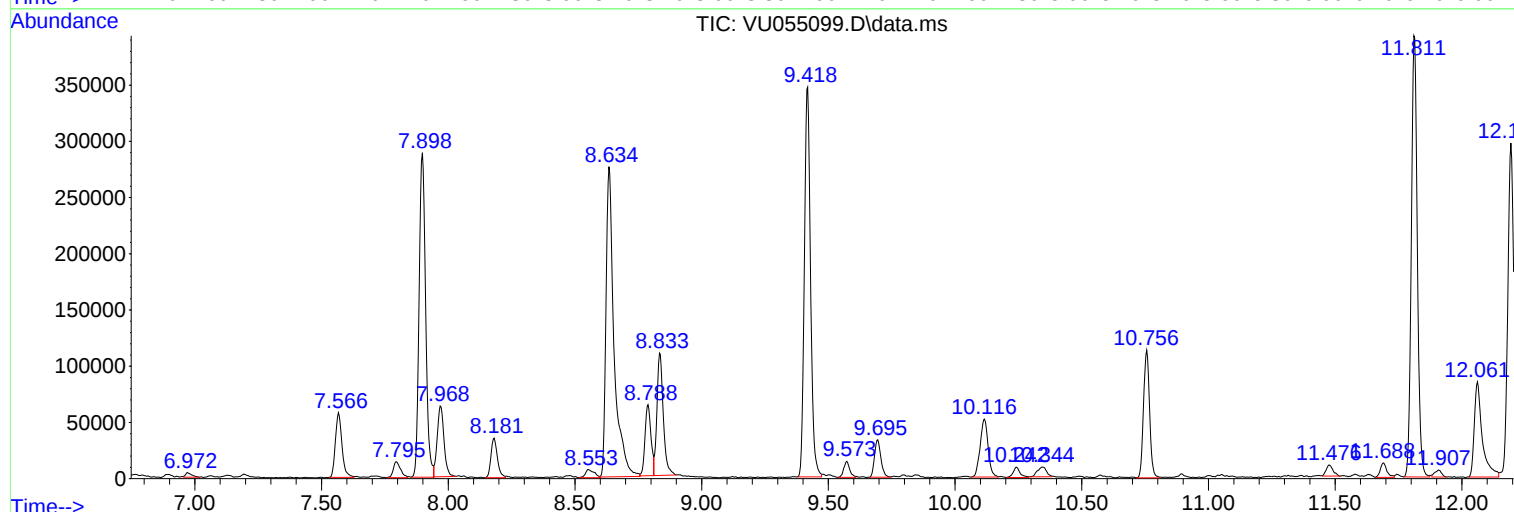
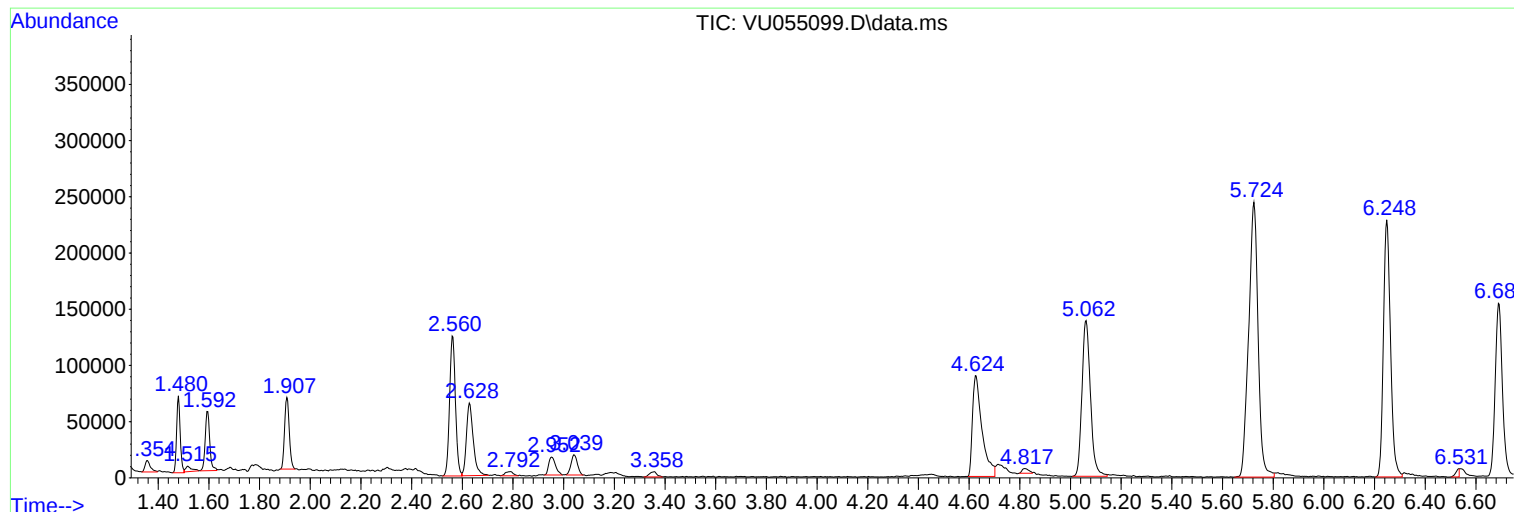
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR090123WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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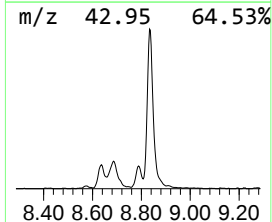
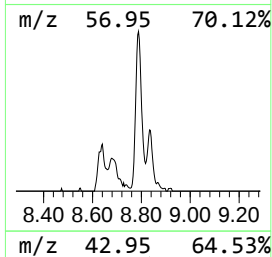
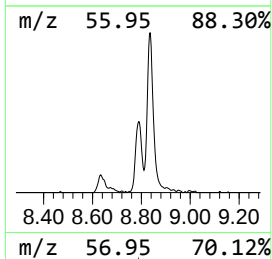
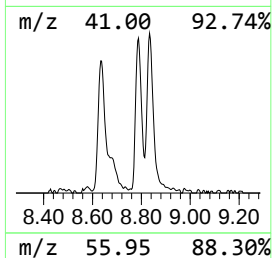
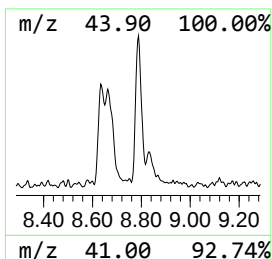
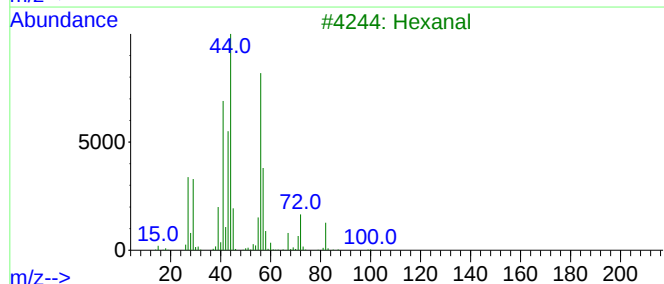
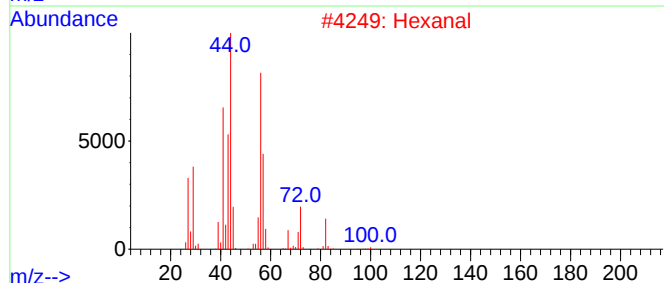
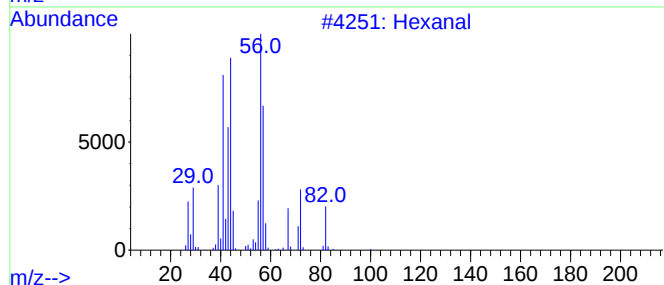
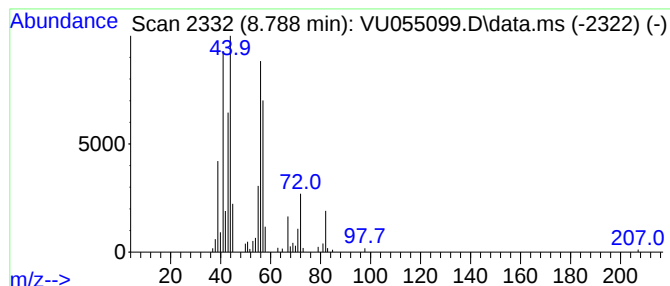
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR090123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Hexanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.788	0.89 ug/L	104881	Chlorobenzene-d5	9.418

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	80
2	Hexanal			100	C6H12O	000066-25-1	72
3	Hexanal			100	C6H12O	000066-25-1	72
4	Hexanal			100	C6H12O	000066-25-1	64
5	Hexanal			100	C6H12O	000066-25-1	59



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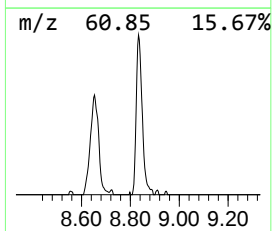
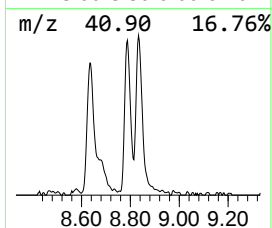
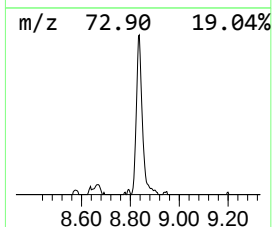
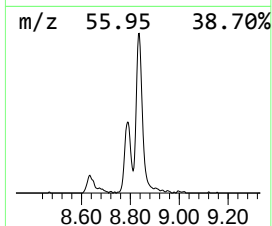
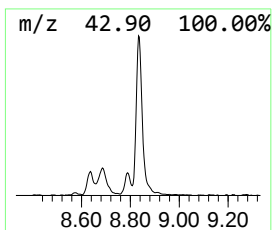
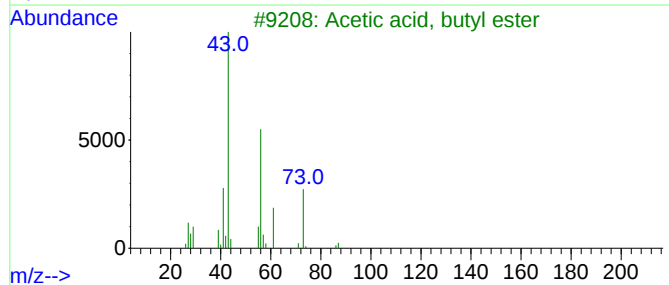
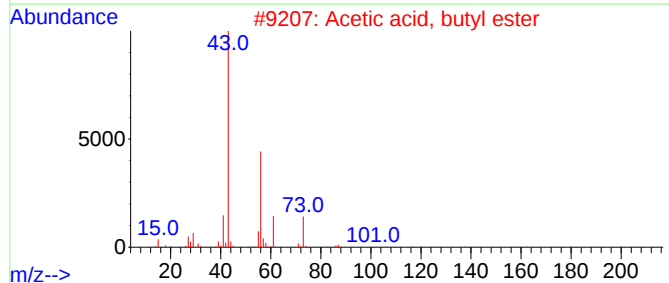
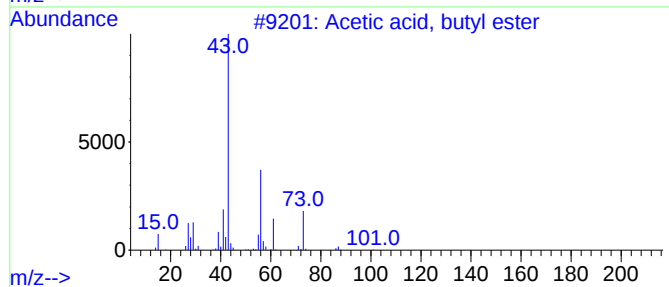
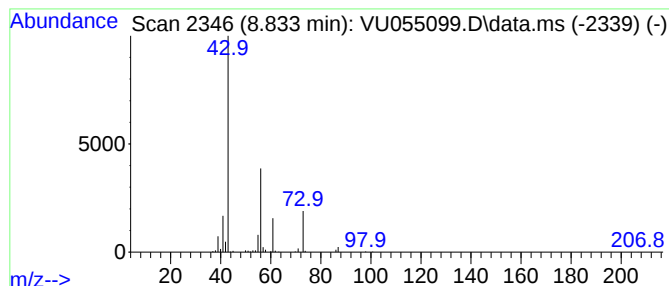
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR090123WMA.M
Quant Title : TRACE VOA SFAM1.0

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	1.58 ug/L	186694	Chlorobenzene-d5	9.418

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester		116	C6H12O2	000123-86-4	78	
2	Acetic acid, butyl ester		116	C6H12O2	000123-86-4	64	
3	Acetic acid, butyl ester		116	C6H12O2	000123-86-4	56	
4	Acetic acid, butyl ester		116	C6H12O2	000123-86-4	40	
5	Isobutylamine		73	C4H11N	000078-81-9	9	



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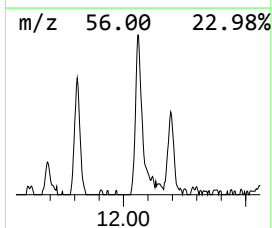
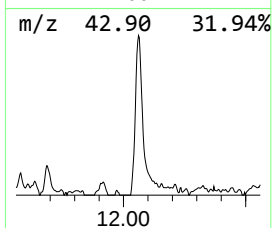
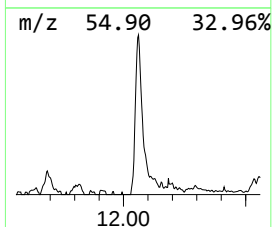
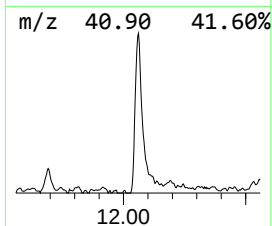
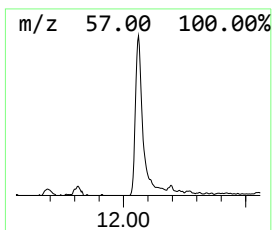
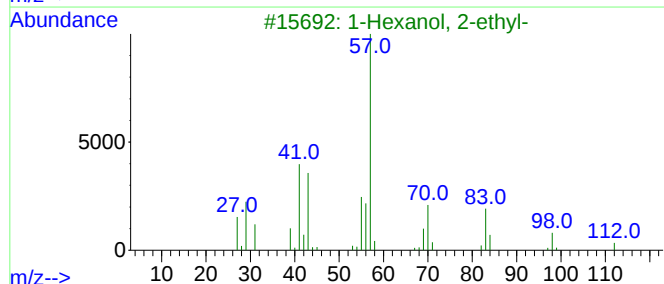
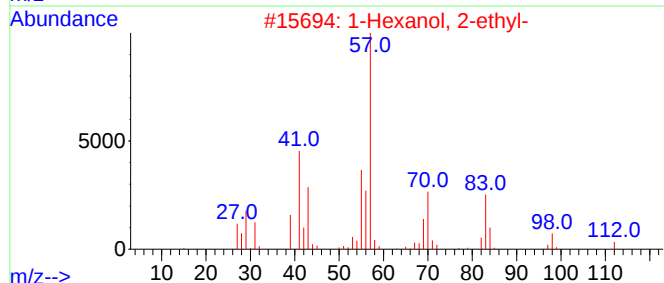
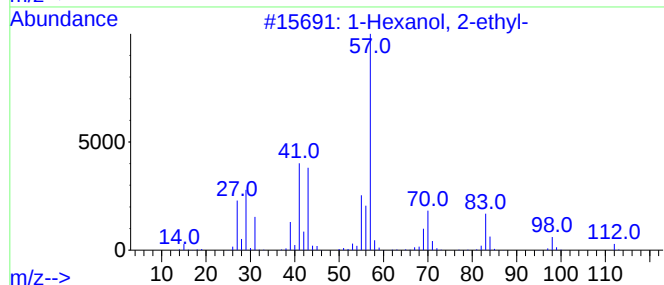
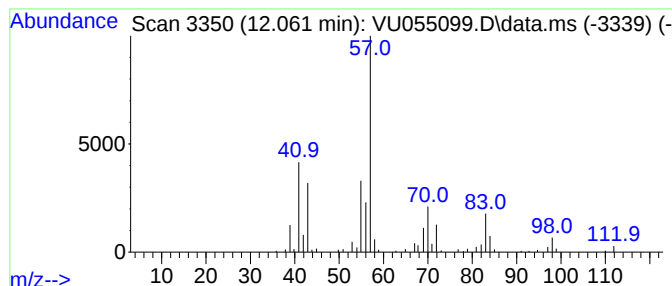
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.061	1.42 ug/L	185190	1,4-Dichlorobenzene-d4	11.814

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	86
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
5	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	59



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanal	8.788	0.9	ug/L	104881	2	9.418	592414	5.0
Acetic acid, bu...	8.833	1.6	ug/L	186694	2	9.418	592414	5.0
1-Hexanol, 2-et...	12.061	1.4	ug/L	185190	3	11.814	650601	5.0