

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW073124\
 Data File : VW029812.D
 Acq On : 31 Jul 2024 13:56
 Operator : SY/MD
 Sample : P3397-01
 Misc : 3.99g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 BHCL0

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

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_W\Method\SFAMWLM072424SMA.M
 Title : SFAM01.0

Signal : TIC: VW029812.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.363	73	78	86	rBV	19285	44476	4.58%	0.614%
2	2.893	160	165	178	rVB2	22560	61324	6.31%	0.847%
3	3.296	229	231	232	rBV2	673	364	0.04%	0.005%
4	3.387	243	246	247	rBV3	746	654	0.07%	0.009%
5	3.503	261	265	266	rBV2	451	710	0.07%	0.010%
6	3.539	269	271	274	rVV2	533	501	0.05%	0.007%
7	3.869	323	325	327	rVB2	432	280	0.03%	0.004%
8	3.917	331	333	334	rBV2	393	280	0.03%	0.004%
9	4.021	340	350	369	rBV2	45625	161320	16.60%	2.228%
10	4.253	386	388	390	rBV3	525	663	0.07%	0.009%
11	4.387	408	410	412	rVB3	486	335	0.03%	0.005%
12	4.417	413	415	416	rBV2	326	219	0.02%	0.003%
13	4.436	416	418	420	rVB3	461	257	0.03%	0.004%
14	4.588	441	443	446	rVB4	460	496	0.05%	0.007%
15	4.618	446	448	450	rBV3	480	358	0.04%	0.005%
16	4.667	454	456	457	rBV2	353	218	0.02%	0.003%
17	4.740	467	468	471	rVB2	399	383	0.04%	0.005%
18	4.923	486	498	522	rVV2	29402	128248	13.19%	1.771%
19	5.118	528	530	531	rBV2	558	422	0.04%	0.006%
20	5.185	538	541	544	rBV4	543	911	0.09%	0.013%
21	5.259	550	553	556	rVB3	361	478	0.05%	0.007%
22	5.313	560	562	564	rBV2	363	408	0.04%	0.006%
23	5.405	574	577	580	rBV4	392	541	0.06%	0.007%
24	5.588	604	607	609	rVB2	532	658	0.07%	0.009%
25	5.618	609	612	615	rBV4	398	709	0.07%	0.010%
26	5.649	615	617	618	rVV2	342	241	0.02%	0.003%
27	5.667	618	620	623	rVB3	526	569	0.06%	0.008%
28	5.722	626	629	630	rBV3	293	273	0.03%	0.004%
29	5.740	630	632	633	rVB	421	261	0.03%	0.004%
30	5.759	633	635	637	rBV3	266	266	0.03%	0.004%
31	5.783	637	639	642	rVV2	459	478	0.05%	0.007%
32	5.832	646	647	650	rVB2	479	340	0.03%	0.005%
33	5.868	650	653	655	rBV3	450	518	0.05%	0.007%
34	5.941	655	665	677	rBV2	9313	29510	3.04%	0.408%
35	6.088	685	689	692	rVB3	896	1055	0.11%	0.015%
36	6.173	701	703	704	rBV2	269	195	0.02%	0.003%

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 Title : SFAM01.0

37	6.277	715	720	723	rBV5	606	960	0.10%	0.013%
38	6.380	734	737	738	rBV3	461	419	0.04%	0.006%
39	6.521	758	760	762	rBV2	471	450	0.05%	0.006%
40	6.545	762	764	768	rVV3	255	318	0.03%	0.004%
41	6.588	768	771	773	rVB	394	495	0.05%	0.007%
42	6.649	777	781	782	rBV2	453	450	0.05%	0.006%
43	6.667	782	784	786	rBV	428	293	0.03%	0.004%
44	6.734	794	795	796	rBV	514	222	0.02%	0.003%
45	6.752	796	798	799	rVV2	465	493	0.05%	0.007%
46	6.789	801	804	806	rBV2	411	524	0.05%	0.007%
47	6.947	828	830	831	rBV	510	370	0.04%	0.005%
48	6.990	836	837	840	rVB2	461	410	0.04%	0.006%
49	7.075	843	851	874	rBV2	42335	148301	15.26%	2.048%
50	7.380	900	901	903	rBV2	428	342	0.04%	0.005%
51	7.508	920	922	923	rBV2	569	466	0.05%	0.006%
52	7.648	935	945	957	rBV	151167	369853	38.05%	5.109%
53	7.929	988	991	992	rBV3	395	334	0.03%	0.005%
54	8.002	1001	1003	1004	rBV2	426	388	0.04%	0.005%
55	8.020	1004	1006	1007	rVV2	391	295	0.03%	0.004%
56	8.075	1013	1015	1018	rVB3	246	253	0.03%	0.003%
57	8.173	1029	1031	1032	rBV	328	216	0.02%	0.003%
58	8.276	1038	1048	1067	rBV2	239683	775057	79.74%	10.706%
59	8.496	1082	1084	1086	rBV3	546	429	0.04%	0.006%
60	8.545	1091	1092	1093	rBV	454	216	0.02%	0.003%
61	8.642	1106	1108	1112	rBV4	475	461	0.05%	0.006%
62	8.673	1112	1113	1114	rBV	797	410	0.04%	0.006%
63	8.776	1127	1130	1131	rBV2	347	253	0.03%	0.003%
64	8.843	1131	1141	1154	rBV	407754	815957	83.95%	11.271%
65	9.075	1175	1179	1188	rVB7	3424	7092	0.73%	0.098%
66	9.270	1201	1211	1221	rBV	212083	433942	44.65%	5.994%
67	9.410	1232	1234	1236	rBV3	324	307	0.03%	0.004%
68	9.666	1270	1276	1284	rBV4	2574	5825	0.60%	0.080%
69	9.874	1308	1310	1313	rVB3	583	527	0.05%	0.007%
70	9.910	1313	1316	1318	rBV2	791	770	0.08%	0.011%
71	10.032	1329	1336	1344	rBV	93299	171518	17.65%	2.369%
72	10.203	1362	1364	1365	rBV	584	442	0.05%	0.006%
73	10.319	1375	1383	1392	rBV	289471	519289	53.43%	7.173%
74	10.520	1415	1416	1418	rBV2	555	347	0.04%	0.005%
75	10.575	1418	1425	1437	rVV	62250	112120	11.54%	1.549%
76	10.697	1440	1445	1450	rBV3	2440	4210	0.43%	0.058%

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 Title : SFAM01.0

77	10.770	1455	1457	1458	rBV	323	203	0.02%	0.003%
78	10.825	1464	1466	1467	rBV	538	420	0.04%	0.006%
79	10.855	1469	1471	1476	rVB5	1773	2757	0.28%	0.038%
80	10.922	1476	1482	1501	rBV	157503	279986	28.81%	3.867%
81	11.392	1552	1559	1562	rBV7	563	1076	0.11%	0.015%
82	11.434	1564	1566	1567	rBV	462	250	0.03%	0.003%
83	11.575	1587	1589	1590	rBV2	253	224	0.02%	0.003%
84	11.629	1590	1598	1607	rBV	575145	971948	100.00%	13.425%
85	11.831	1628	1631	1635	rBV5	975	1459	0.15%	0.020%
86	11.928	1646	1647	1648	rBV	362	253	0.03%	0.003%
87	12.093	1669	1674	1681	rBV	3581	6201	0.64%	0.086%
88	12.452	1732	1733	1735	rBV2	525	345	0.04%	0.005%
89	12.556	1747	1750	1752	rBV3	575	766	0.08%	0.011%
90	12.690	1765	1772	1781	rBV	213462	355600	36.59%	4.912%
91	12.879	1799	1803	1804	rBV2	930	1196	0.12%	0.017%
92	13.117	1837	1842	1847	rBV3	5414	8558	0.88%	0.118%
93	13.300	1867	1872	1878	rVB	20384	31160	3.21%	0.430%
94	13.556	1906	1914	1923	rBV	539517	859616	88.44%	11.874%
95	13.641	1923	1928	1942	rVB	104636	176678	18.18%	2.440%
96	13.849	1955	1962	1972	rBV	368087	599961	61.73%	8.287%
97	14.519	2066	2072	2084	rBV	67553	114379	11.77%	1.580%
98	15.245	2187	2191	2198	rVB3	7316	12069	1.24%	0.167%
99	16.263	2357	2358	2359	rBV	693	362	0.04%	0.005%
100	16.299	2363	2364	2365	rBV	403	268	0.03%	0.004%

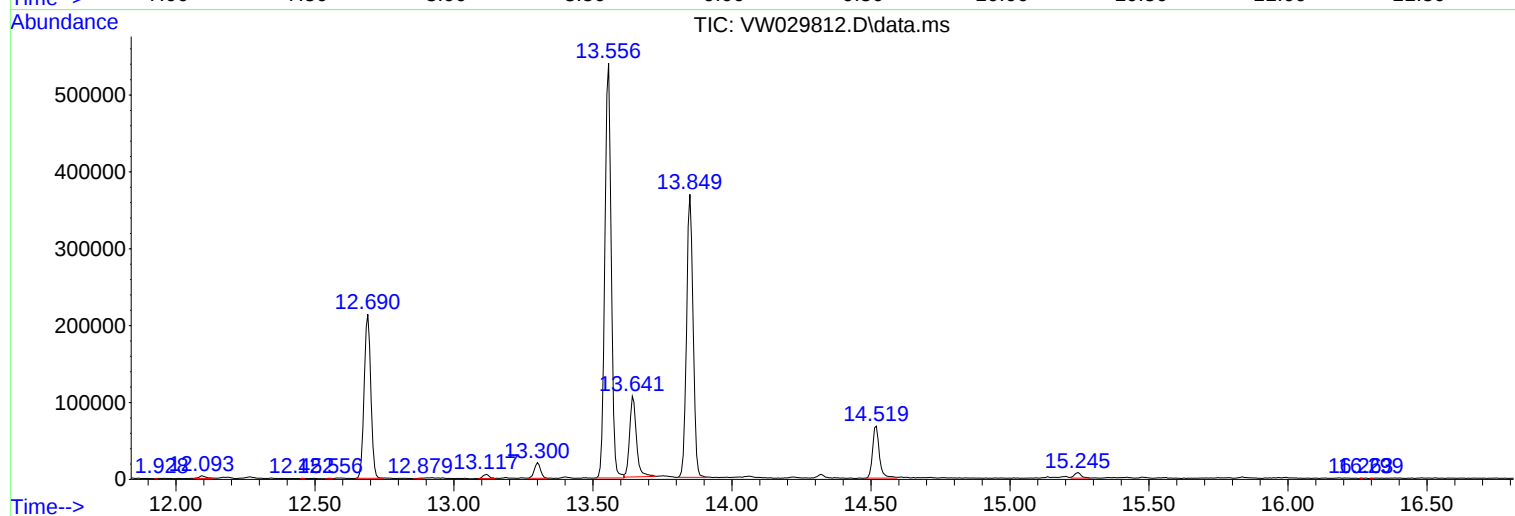
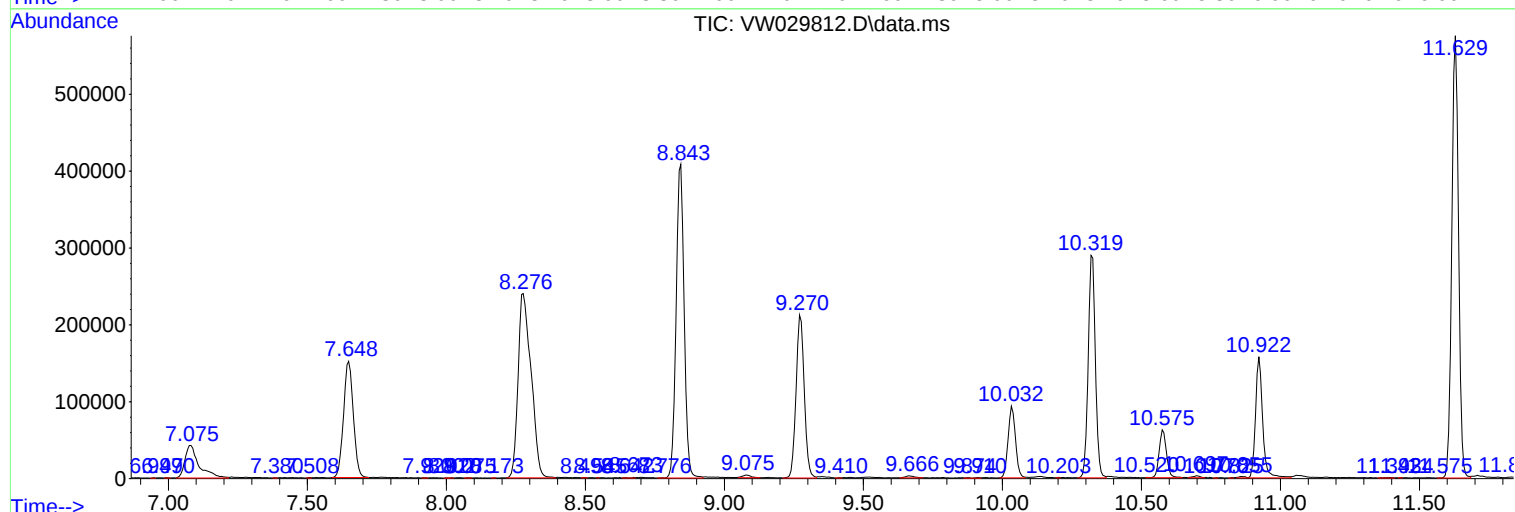
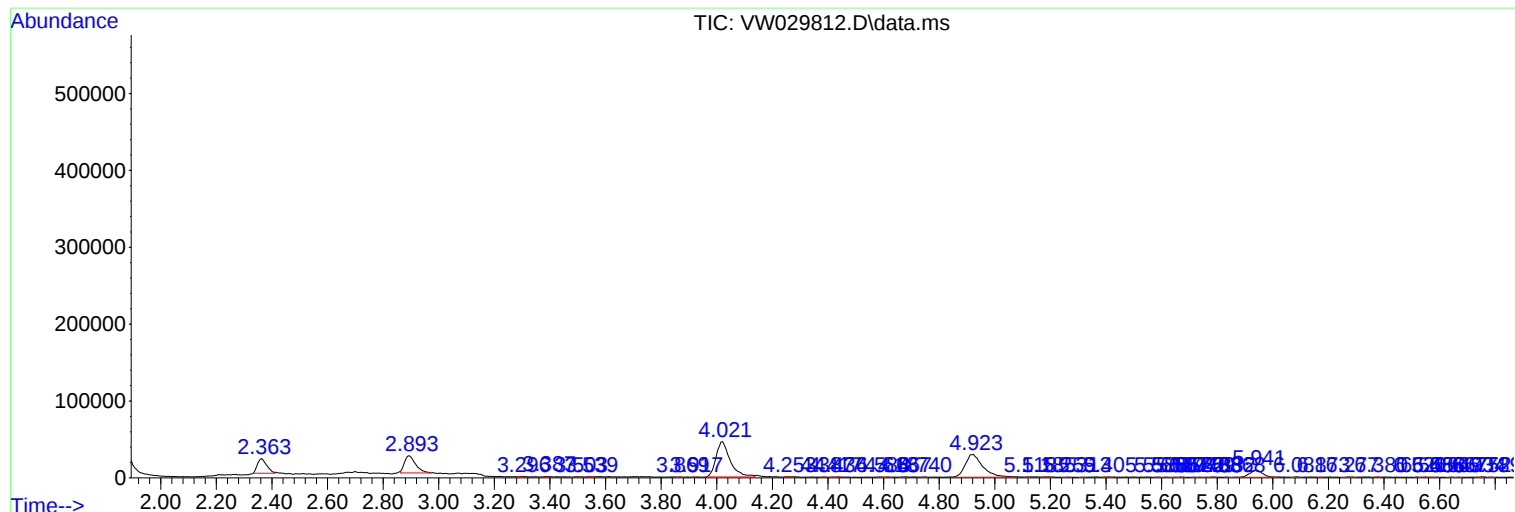
Sum of corrected areas: 7239678

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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



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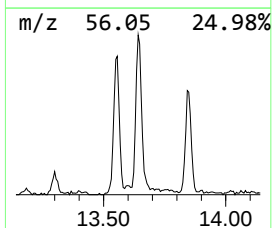
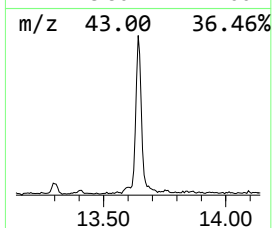
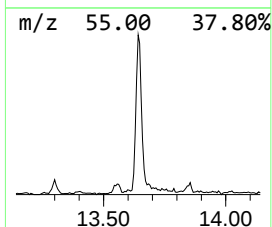
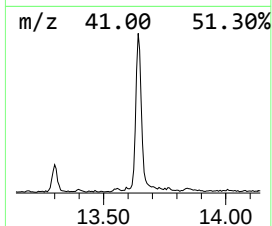
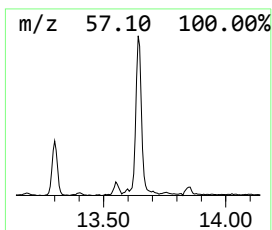
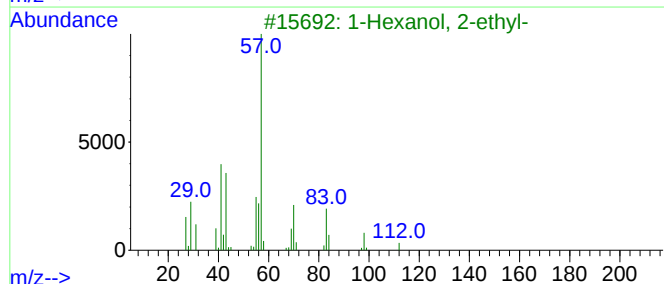
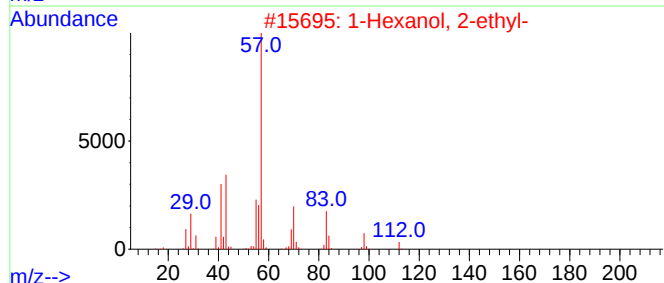
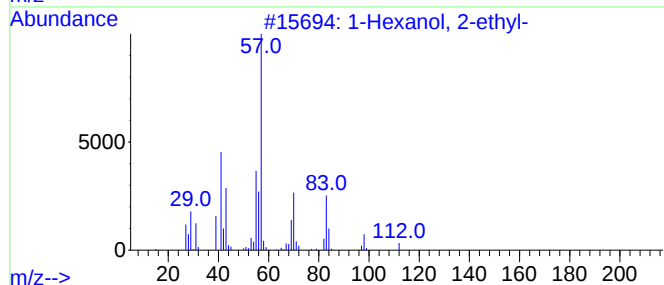
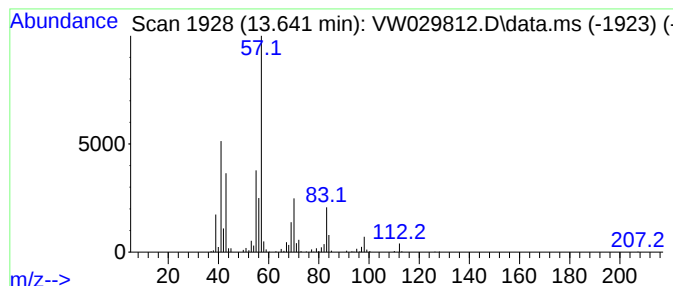
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.641	5.14 ug/L	176678	1,4-Dichlorobenzene-d4	13.556

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
4		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	64



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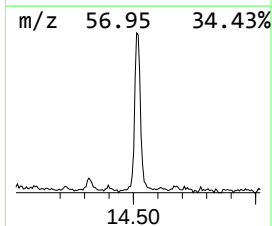
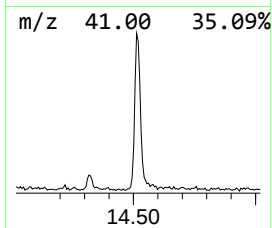
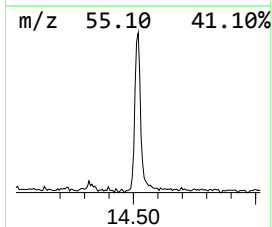
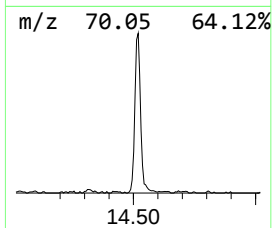
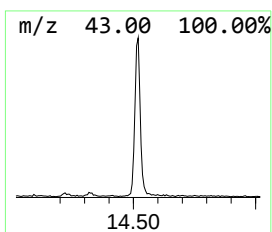
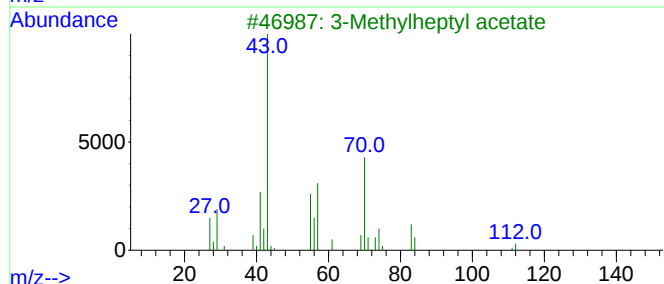
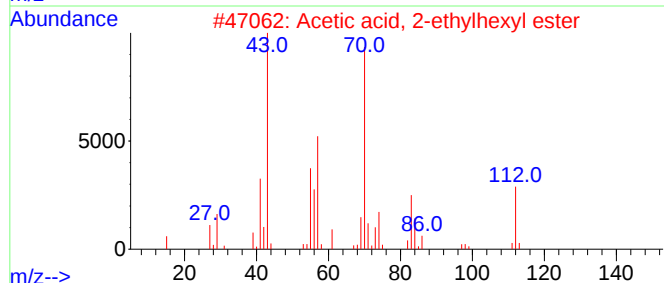
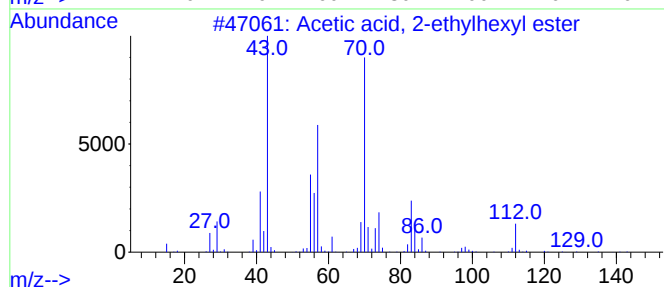
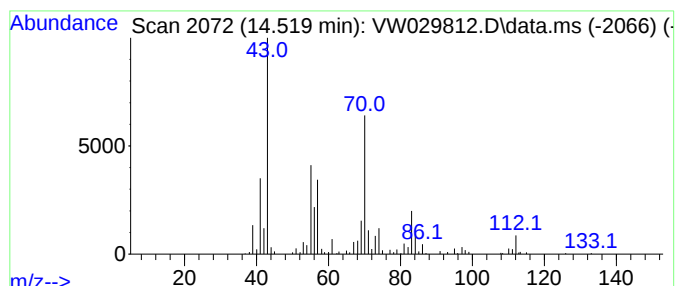
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 Acetic acid, 2-ethylhexyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.519	3.33 ug/L	114379	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	91		
2	Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	90		
3	3-Methylheptyl acetate	172	C10H20O2	072218-58-7	83		
4	Acetic acid, 2-ethylhexyl ester	172	C10H20O2	000103-09-3	78		
5	2-Ethylhexyl acrylate	184	C11H20O2	000103-11-7	72		



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Quant Title : SFAM01.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	13.641	5.1	ug/L	176678	3	13.556	859616	25.0
Acetic acid, 2-...	14.519	3.3	ug/L	114379	3	13.556	859616	25.0