

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW082724\
 Data File : VW030062.D
 Acq On : 27 Aug 2024 23:58
 Operator : SY/MD
 Sample : P3733-07
 Misc : 6.17g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 A44A1

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\SFAMWLM082624SMA.M
 Title : SFAM01.0

Signal : TIC: VW030062.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	71	78	96	rBV	38853	110667	16.10%	2.783%
2	2.893	158	165	182	rBV	32754	92750	13.49%	2.332%
3	3.686	293	295	298	rVB2	218	169	0.02%	0.004%
4	3.716	298	300	301	rBV	214	186	0.03%	0.005%
5	3.783	307	311	314	rBV2	224	389	0.06%	0.010%
6	3.911	328	332	334	rBV2	158	199	0.03%	0.005%
7	4.021	337	350	363	rBV	69026	245686	35.73%	6.178%
8	4.387	405	410	411	rBV2	360	528	0.08%	0.013%
9	4.655	451	454	455	rBV2	283	307	0.04%	0.008%
10	4.740	466	468	473	rVB3	192	208	0.03%	0.005%
11	4.795	475	477	480	rVB	278	216	0.03%	0.005%
12	4.923	487	498	517	rBV3	6321	24695	3.59%	0.621%
13	5.124	530	531	534	rVB2	253	193	0.03%	0.005%
14	5.191	538	542	543	rBV3	252	285	0.04%	0.007%
15	5.228	546	548	550	rVV	255	181	0.03%	0.005%
16	5.271	554	555	557	rBV2	223	181	0.03%	0.005%
17	5.429	579	581	585	rVB	336	273	0.04%	0.007%
18	5.575	604	605	610	rBV2	199	290	0.04%	0.007%
19	5.777	636	638	639	rBV2	423	327	0.05%	0.008%
20	5.935	656	664	675	rVB5	3074	9455	1.38%	0.238%
21	6.112	688	693	694	rBV2	386	380	0.06%	0.010%
22	6.911	817	824	834	rBV4	1170	3482	0.51%	0.088%
23	6.984	834	836	837	rBV	374	320	0.05%	0.008%
24	7.087	844	853	862	rBV	23116	68466	9.96%	1.722%
25	7.648	934	945	956	rBV	118783	300219	43.66%	7.550%
26	7.770	962	965	967	rVB	163	163	0.02%	0.004%
27	7.874	973	982	995	rBV	18189	47192	6.86%	1.187%
28	7.965	995	997	1001	rVB2	345	352	0.05%	0.009%
29	8.008	1001	1004	1005	rBV3	180	204	0.03%	0.005%
30	8.093	1014	1018	1021	rVB2	164	265	0.04%	0.007%
31	8.276	1037	1048	1065	rVV2	233149	687551	100.00%	17.290%
32	8.557	1087	1094	1103	rBV4	1699	4323	0.63%	0.109%
33	8.709	1112	1119	1126	rBV3	1363	2820	0.41%	0.071%
34	8.843	1132	1141	1155	rVB	223455	448152	65.18%	11.270%
35	8.977	1160	1163	1164	rVV2	243	260	0.04%	0.007%
36	9.008	1164	1168	1169	rVB	255	237	0.03%	0.006%

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 Title : SFAM01.0

37	9.075	1178	1179	1181	rBV	330	225	0.03%	0.006%
38	9.270	1203	1211	1223	rBV	159589	331957	48.28%	8.348%
39	9.410	1228	1234	1243	rBV3	3891	8543	1.24%	0.215%
40	9.544	1253	1256	1260	rBV3	231	304	0.04%	0.008%
41	9.642	1270	1272	1274	rBV	280	251	0.04%	0.006%
42	9.806	1297	1299	1303	rVB2	212	230	0.03%	0.006%
43	9.849	1303	1306	1309	rBV2	167	227	0.03%	0.006%
44	10.032	1328	1336	1346	rBV	70588	129414	18.82%	3.254%
45	10.215	1363	1366	1369	rVV2	667	862	0.13%	0.022%
46	10.318	1376	1383	1403	rVB	227195	415353	60.41%	10.445%
47	10.575	1417	1425	1432	rBV	42731	75834	11.03%	1.907%
48	10.703	1441	1446	1452	rVB2	5985	9901	1.44%	0.249%
49	10.782	1457	1459	1462	rBV2	220	240	0.03%	0.006%
50	10.861	1465	1472	1476	rBV2	9316	17139	2.49%	0.431%
51	10.922	1476	1482	1496	rVV	92931	165023	24.00%	4.150%
52	11.068	1500	1506	1516	rVB3	10335	19221	2.80%	0.483%
53	11.410	1561	1562	1565	rBV	136	161	0.02%	0.004%
54	11.471	1568	1572	1573	rBV	190	228	0.03%	0.006%
55	11.538	1580	1583	1586	rVV2	178	251	0.04%	0.006%
56	11.568	1586	1588	1591	rVV	154	172	0.03%	0.004%
57	11.629	1591	1598	1612	rVV	191055	321991	46.83%	8.097%
58	11.727	1612	1614	1617	rVB3	576	492	0.07%	0.012%
59	11.849	1628	1634	1644	rVV2	5949	13289	1.93%	0.334%
60	11.940	1646	1649	1655	rVB3	1678	2913	0.42%	0.073%
61	12.166	1681	1686	1688	rBV3	213	341	0.05%	0.009%
62	12.239	1695	1698	1704	rBV2	357	415	0.06%	0.010%
63	12.336	1709	1714	1719	rBV3	2833	5040	0.73%	0.127%
64	12.562	1749	1751	1752	rBV	260	173	0.03%	0.004%
65	12.599	1752	1757	1765	rVB2	6741	10434	1.52%	0.262%
66	12.690	1765	1772	1780	rBV	94385	157181	22.86%	3.953%
67	12.751	1780	1782	1789	rVB3	641	780	0.11%	0.020%
68	12.885	1803	1804	1806	rBV	297	311	0.05%	0.008%
69	13.044	1827	1830	1834	rBV3	621	802	0.12%	0.020%
70	13.092	1836	1838	1840	rBV2	152	162	0.02%	0.004%
71	13.159	1846	1849	1851	rBV2	209	214	0.03%	0.005%
72	13.226	1856	1860	1862	rBV2	139	166	0.02%	0.004%
73	13.275	1862	1868	1875	rBV3	1995	4247	0.62%	0.107%
74	13.391	1883	1887	1891	rBV4	1275	2085	0.30%	0.052%
75	13.556	1907	1914	1922	rVB	67895	110488	16.07%	2.779%
76	13.641	1924	1928	1935	rVB	8970	14119	2.05%	0.355%

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 Title : SFAM01.0

77	13.848	1955	1962	1973	rVB	54228	90362	13.14%	2.272%
78	14.019	1987	1990	1992	rVB	277	247	0.04%	0.006%
79	14.062	1992	1997	2003	rBV2	2092	3328	0.48%	0.084%
80	14.171	2011	2015	2017	rBV	164	238	0.03%	0.006%
81	14.226	2020	2024	2025	rBV2	304	340	0.05%	0.009%
82	14.269	2029	2031	2032	rVB	233	169	0.02%	0.004%
83	14.324	2035	2040	2044	rVB3	2107	2975	0.43%	0.075%
84	14.421	2054	2056	2058	rBV3	179	169	0.02%	0.004%
85	14.482	2064	2066	2069	rBV2	126	167	0.02%	0.004%
86	14.513	2069	2071	2076	rVB3	367	556	0.08%	0.014%
87	14.616	2085	2088	2091	rBV3	171	192	0.03%	0.005%
88	14.757	2109	2111	2113	rBV	168	203	0.03%	0.005%
89	14.830	2121	2123	2125	rBV2	270	293	0.04%	0.007%
90	15.122	2169	2171	2174	rVB2	234	187	0.03%	0.005%
91	15.153	2174	2176	2178	rBV2	356	285	0.04%	0.007%
92	15.220	2185	2187	2190	rBV2	193	245	0.04%	0.006%
93	15.476	2224	2229	2237	rVB3	967	1883	0.27%	0.047%
94	15.787	2278	2280	2284	rBV2	361	250	0.04%	0.006%
95	15.909	2298	2300	2302	rBV	252	274	0.04%	0.007%
96	16.013	2316	2317	2319	rBV	314	220	0.03%	0.006%
97	16.067	2323	2326	2327	rBV2	266	309	0.04%	0.008%
98	16.305	2363	2365	2366	rBV	406	277	0.04%	0.007%
99	16.336	2368	2370	2373	rBV2	277	240	0.03%	0.006%
100	16.445	2387	2388	2391	rBV2	299	319	0.05%	0.008%

Sum of corrected areas: 3976478

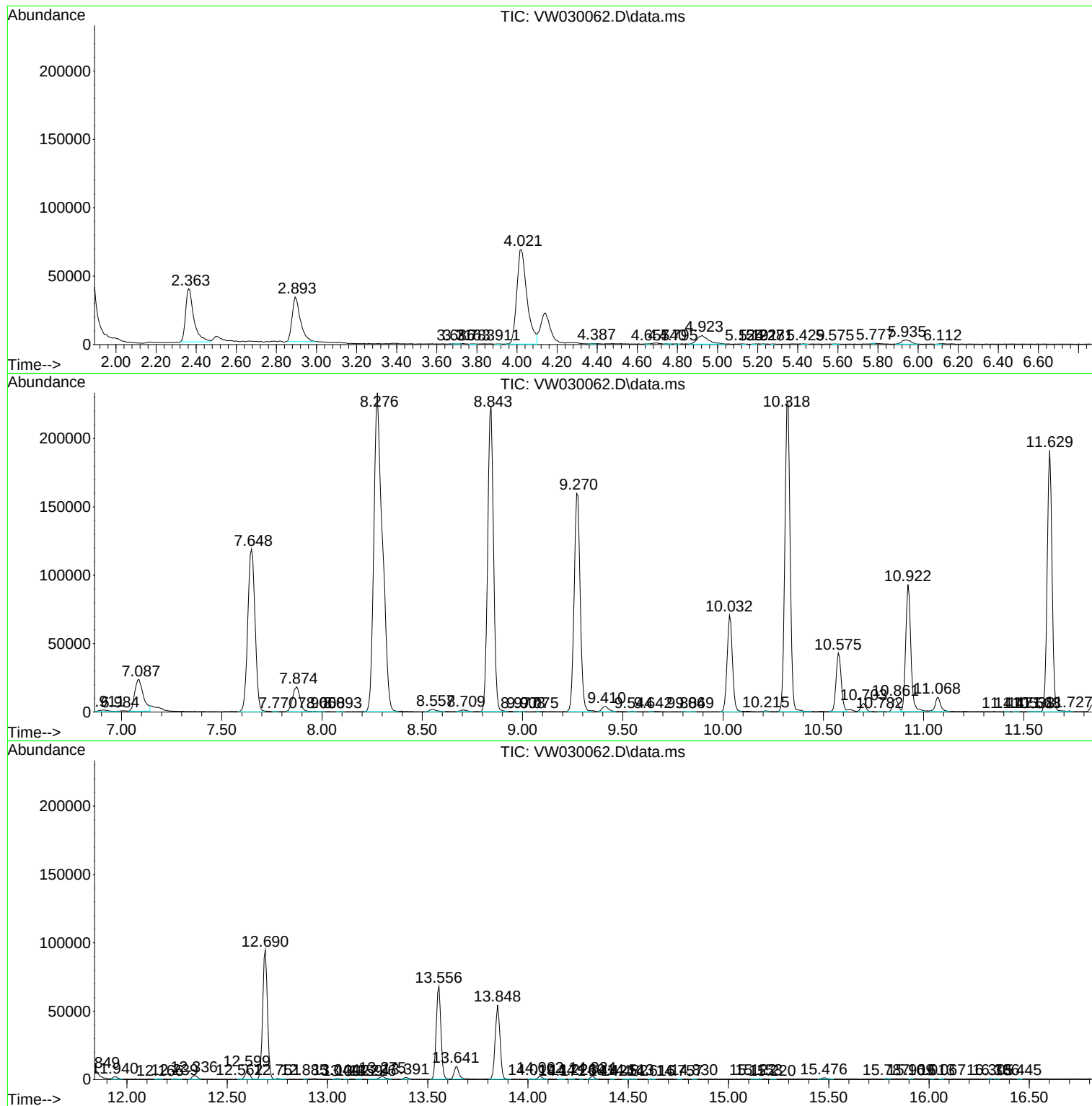
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM082624SMA.M
Quant Title : SFAM01.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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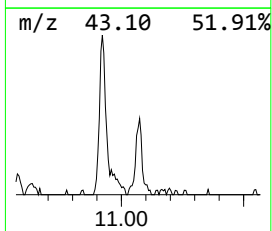
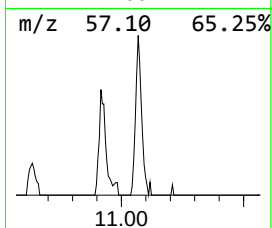
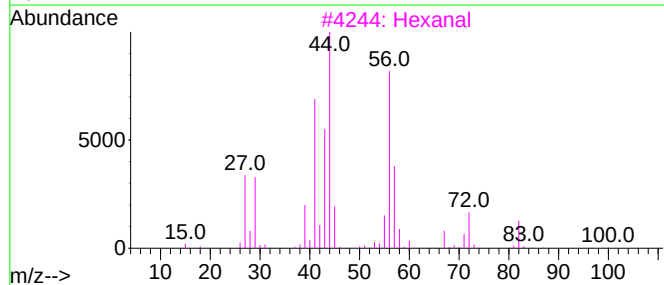
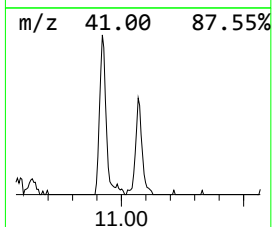
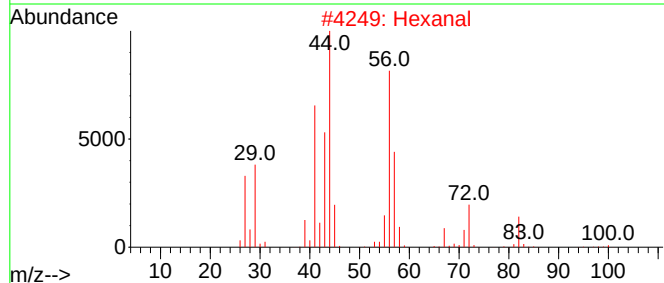
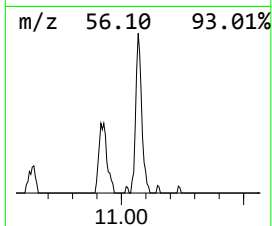
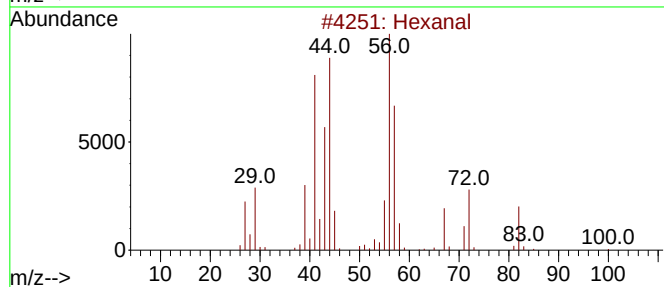
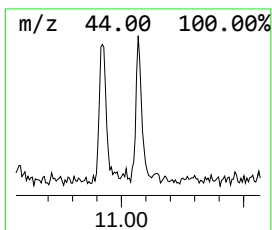
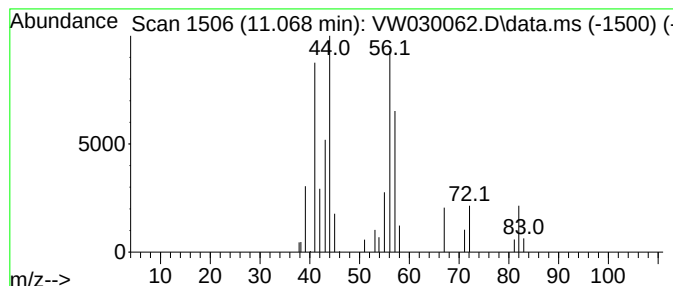
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM082624SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 Hexanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.068	1.49 ug/L	19221	Chlorobenzene-d5	11.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	86
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	64



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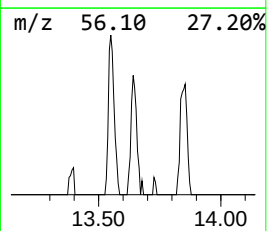
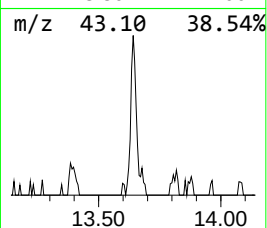
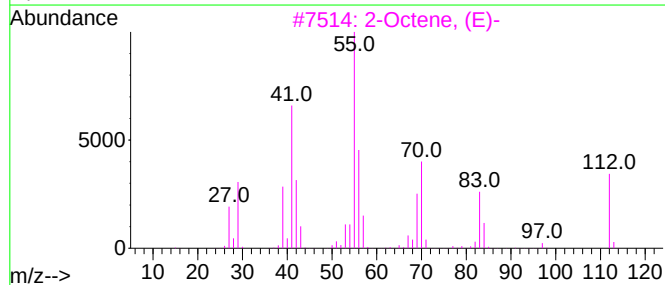
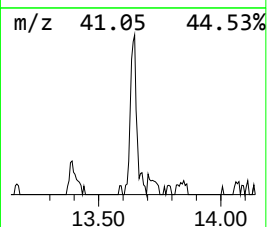
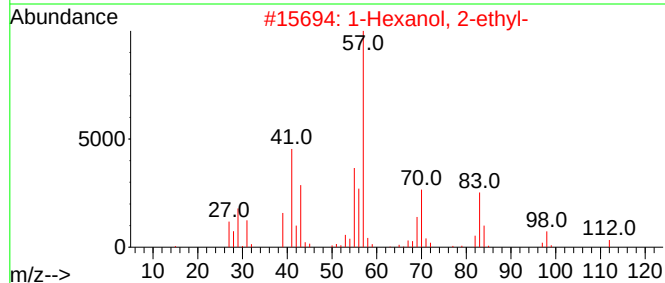
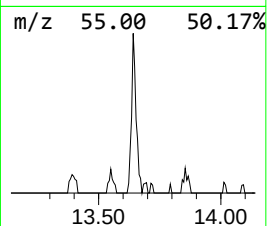
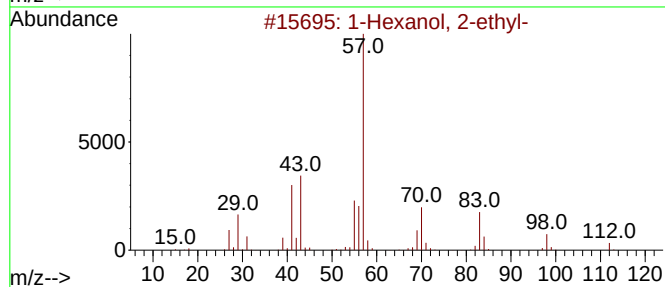
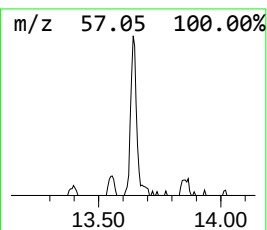
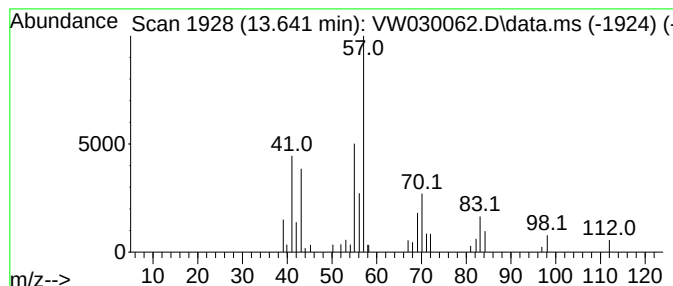
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM082624SMA.M
Quant Title : SFAM01.0

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.641	3.19 ug/L	14119	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	78
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
3	2-Octene, (E)-			112	C8H16	013389-42-9	64
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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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanal	11.068	1.5	ug/L	19221	2	11.629	321991	25.0
1-Hexanol, 2-et...	13.641	3.2	ug/L	14119	3	13.556	110488	25.0