

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW101821\
 Data File : VW020561.D
 Acq On : 18 Oct 2021 14:32
 Operator : SY/VA
 Sample : M4211-06
 Misc : 5.85g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 JDGA5

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\SFAMWLM100821SMA.M
 Title : SFAM01.0

Signal : TIC: VW020561.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.343	67	72	82	rVB	69750	113708	12.11%	1.744%
2	2.873	153	159	171	rVB	32479	63400	6.75%	0.972%
3	4.013	335	346	359	rVV	98186	291074	31.01%	4.464%
4	4.123	361	364	375	rVB2	2398	6526	0.70%	0.100%
5	4.202	375	377	379	rBV	171	113	0.01%	0.002%
6	4.233	381	382	383	rBV	327	219	0.02%	0.003%
7	4.367	401	404	406	rBV	206	274	0.03%	0.004%
8	4.507	420	427	432	rVB3	677	1607	0.17%	0.025%
9	4.672	449	454	456	rVV3	141	152	0.02%	0.002%
10	4.696	456	458	460	rBV2	164	139	0.01%	0.002%
11	4.922	482	495	506	rBV3	9034	29838	3.18%	0.458%
12	5.025	511	512	514	rBV	140	110	0.01%	0.002%
13	5.178	533	537	539	rBV2	103	136	0.01%	0.002%
14	5.263	549	551	554	rVB2	127	120	0.01%	0.002%
15	5.306	554	558	559	rBV2	95	127	0.01%	0.002%
16	5.397	571	573	576	rBV	129	140	0.01%	0.002%
17	5.873	647	651	652	rVB2	81	109	0.01%	0.002%
18	5.934	652	661	670	rBV4	2124	6393	0.68%	0.098%
19	6.147	693	696	697	rBV	101	105	0.01%	0.002%
20	6.178	700	701	704	rVB	147	123	0.01%	0.002%
21	6.208	704	706	709	rBV	97	112	0.01%	0.002%
22	6.818	803	806	808	rBV2	97	126	0.01%	0.002%
23	6.879	815	816	819	rVB2	142	123	0.01%	0.002%
24	7.080	841	849	867	rBV	28350	78446	8.36%	1.203%
25	7.373	895	897	899	rVB2	153	111	0.01%	0.002%
26	7.391	899	900	904	rBV2	91	136	0.01%	0.002%
27	7.555	920	927	932	rVB4	298	740	0.08%	0.011%
28	7.647	932	942	959	rBV	161240	397311	42.32%	6.093%
29	7.952	991	992	995	rVV	186	161	0.02%	0.002%
30	8.031	997	1005	1008	rVB2	125	196	0.02%	0.003%
31	8.275	1035	1045	1059	rBV2	321622	938741	100.00%	14.397%
32	8.689	1110	1113	1117	rVB2	317	347	0.04%	0.005%
33	8.842	1130	1138	1153	rBV	315033	604976	64.45%	9.278%
34	8.994	1160	1163	1166	rVB2	127	161	0.02%	0.002%
35	9.037	1166	1170	1172	rBV2	753	1053	0.11%	0.016%
36	9.122	1181	1184	1186	rBV2	139	124	0.01%	0.002%

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 Title : SFAM01.0

37	9.275	1200	1209	1222	rBV	225252	458181	48.81%	7.027%
38	9.415	1230	1232	1234	rBV	292	230	0.02%	0.004%
39	9.512	1245	1248	1249	rBV2	131	164	0.02%	0.003%
40	9.665	1268	1273	1278	rVB2	791	1264	0.13%	0.019%
41	10.037	1326	1334	1342	rBV	109715	197756	21.07%	3.033%
42	10.244	1367	1368	1371	rBV3	119	127	0.01%	0.002%
43	10.323	1373	1381	1388	rBV	429767	742548	79.10%	11.388%
44	10.390	1388	1392	1398	rVB	6677	11169	1.19%	0.171%
45	10.451	1401	1402	1407	rVB2	150	145	0.02%	0.002%
46	10.500	1407	1410	1414	rVB3	266	401	0.04%	0.006%
47	10.579	1416	1423	1435	rBV	76120	125509	13.37%	1.925%
48	10.707	1439	1444	1448	rBV2	4332	7635	0.81%	0.117%
49	10.835	1461	1465	1470	rBV2	220	401	0.04%	0.006%
50	10.927	1473	1480	1494	rVV	106657	182250	19.41%	2.795%
51	11.073	1498	1504	1511	rVB3	7741	14298	1.52%	0.219%
52	11.171	1518	1520	1526	rVB2	226	282	0.03%	0.004%
53	11.494	1569	1573	1575	rBV2	117	134	0.01%	0.002%
54	11.567	1582	1585	1588	rBV2	117	128	0.01%	0.002%
55	11.634	1588	1596	1607	rBV	406505	691321	73.64%	10.602%
56	11.841	1625	1630	1634	rVV4	629	1233	0.13%	0.019%
57	12.018	1652	1659	1670	rBV	4982	9193	0.98%	0.141%
58	12.170	1678	1684	1689	rVB4	591	1095	0.12%	0.017%
59	12.231	1692	1694	1698	rVB2	253	374	0.04%	0.006%
60	12.280	1698	1702	1704	rBV2	178	167	0.02%	0.003%
61	12.341	1707	1712	1719	rBV2	4977	7841	0.84%	0.120%
62	12.463	1730	1732	1735	rBV2	174	190	0.02%	0.003%
63	12.603	1748	1755	1760	rBV3	3403	5792	0.62%	0.089%
64	12.689	1763	1769	1777	rVV	148128	247725	26.39%	3.799%
65	12.750	1777	1779	1785	rVV2	414	641	0.07%	0.010%
66	12.811	1787	1789	1792	rVV	124	166	0.02%	0.003%
67	12.865	1792	1798	1799	rVV2	192	266	0.03%	0.004%
68	12.932	1803	1809	1814	rVB5	1676	2636	0.28%	0.040%
69	13.042	1822	1827	1828	rBV3	1076	1349	0.14%	0.021%
70	13.079	1829	1833	1838	rVV2	6454	9950	1.06%	0.153%
71	13.134	1838	1842	1848	rVB2	2368	3883	0.41%	0.060%
72	13.243	1858	1860	1862	rBV3	488	454	0.05%	0.007%
73	13.286	1863	1867	1872	rVV2	8460	13612	1.45%	0.209%
74	13.335	1872	1875	1880	rVV	3356	4566	0.49%	0.070%
75	13.396	1880	1885	1891	rVB2	3466	5911	0.63%	0.091%
76	13.481	1896	1899	1900	rBV2	236	229	0.02%	0.004%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM100821SMA.M
 Title : SFAM01.0

77	13.499	1900	1902	1903	rBV2	173	129	0.01%	0.002%
78	13.554	1904	1911	1918	rBV	348328	561766	59.84%	8.616%
79	13.646	1921	1926	1940	rVB	26475	41571	4.43%	0.638%
80	13.853	1953	1960	1967	rBV	324008	512637	54.61%	7.862%
81	14.018	1979	1987	1991	rBV3	6459	13822	1.47%	0.212%
82	14.066	1992	1995	2001	rVB	5151	7869	0.84%	0.121%
83	14.133	2004	2006	2007	rBV2	403	361	0.04%	0.006%
84	14.322	2033	2037	2047	rVB4	7973	13636	1.45%	0.209%
85	14.420	2050	2053	2058	rVB3	656	900	0.10%	0.014%
86	14.658	2090	2092	2094	rBV	211	190	0.02%	0.003%
87	14.719	2100	2102	2106	rBV4	406	505	0.05%	0.008%
88	14.774	2107	2111	2115	rVV2	1506	2128	0.23%	0.033%
89	14.865	2119	2126	2133	rBV	17050	28014	2.98%	0.430%
90	14.950	2135	2140	2151	rVB	16854	28241	3.01%	0.433%
91	15.066	2156	2159	2170	rVB3	1647	2856	0.30%	0.044%
92	15.243	2184	2188	2194	rBV6	596	1187	0.13%	0.018%
93	15.322	2199	2201	2204	rVB3	253	272	0.03%	0.004%
94	15.395	2211	2213	2214	rBV2	514	504	0.05%	0.008%
95	15.438	2215	2220	2224	rVV3	3290	5387	0.57%	0.083%
96	15.487	2224	2228	2232	rVB2	1640	2440	0.26%	0.037%
97	15.847	2282	2287	2297	rVB3	1376	2733	0.29%	0.042%
98	16.237	2350	2351	2354	rBV	309	215	0.02%	0.003%
99	16.365	2367	2372	2377	rVB5	1036	1691	0.18%	0.026%
100	16.438	2379	2384	2390	rVB4	1398	2848	0.30%	0.044%

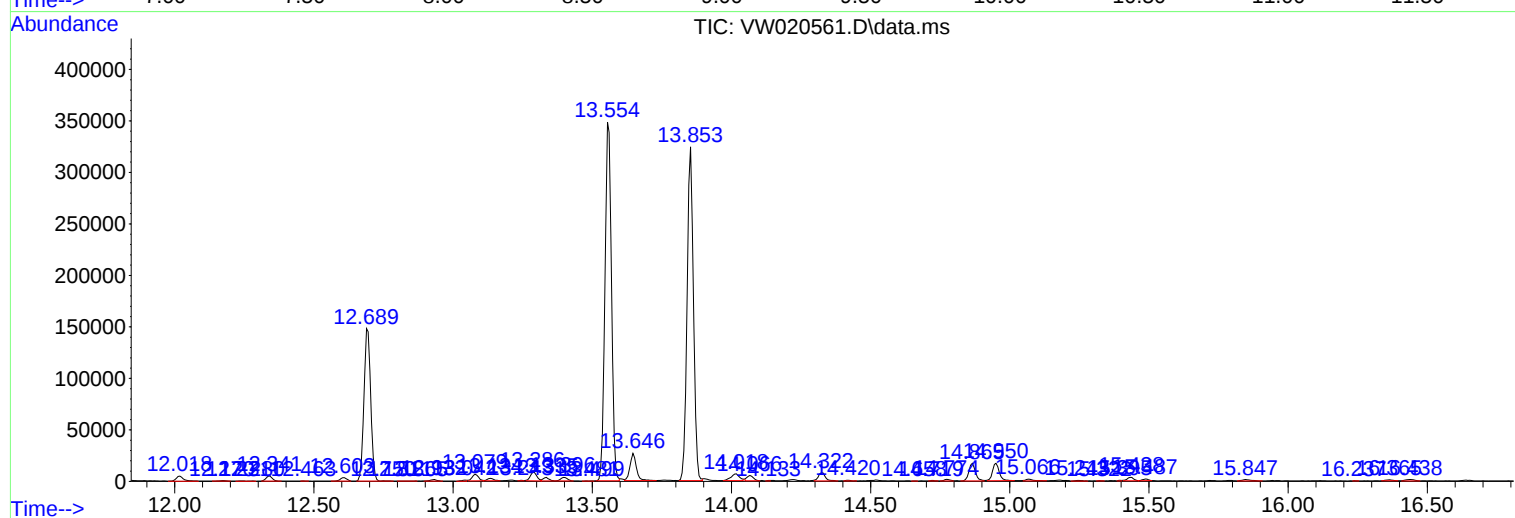
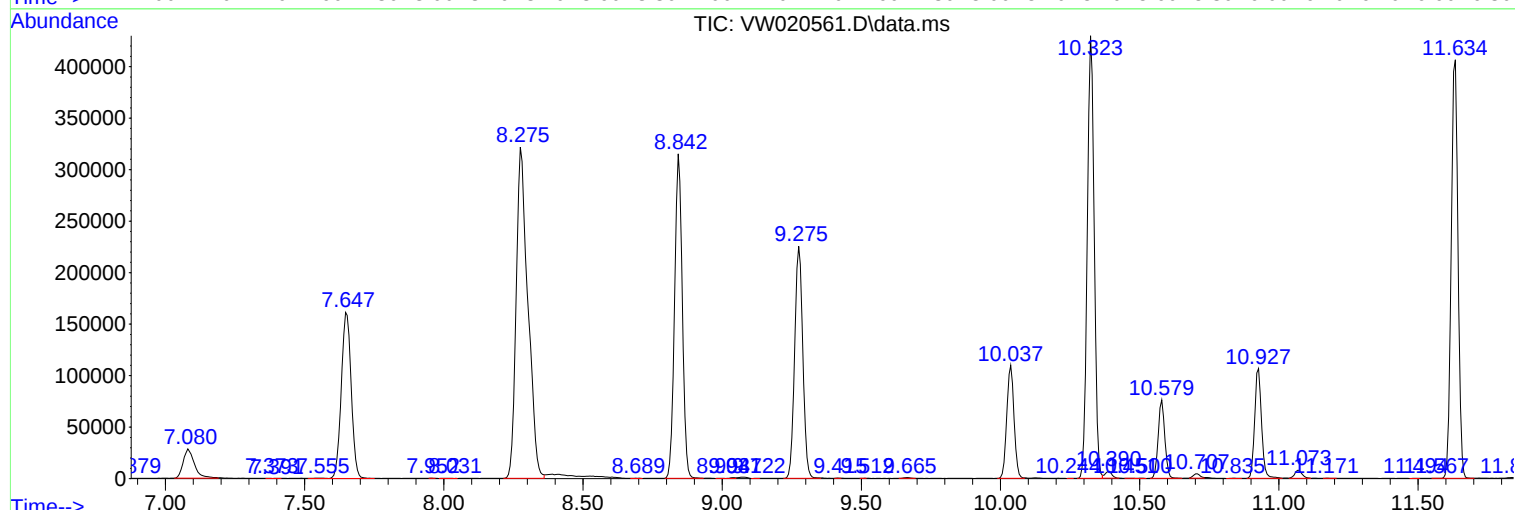
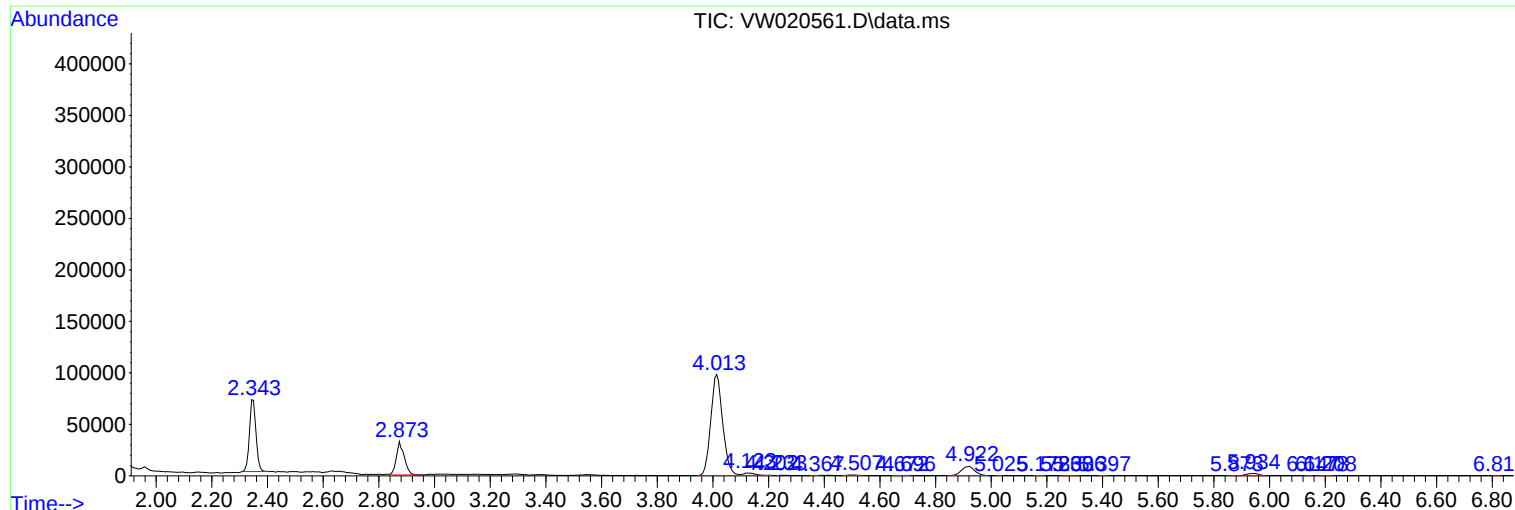
Sum of corrected areas: 6520395

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM100821SMA.M
Quant Title : SFAM01.0

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



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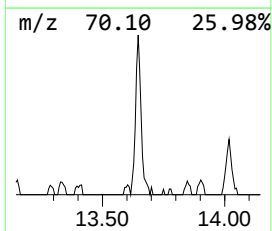
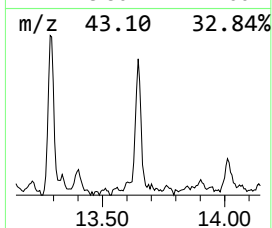
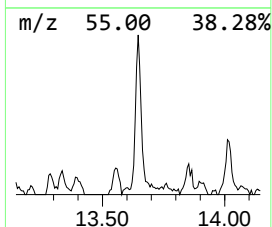
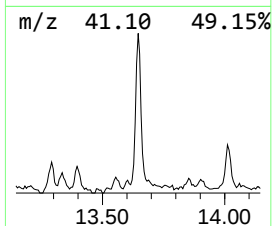
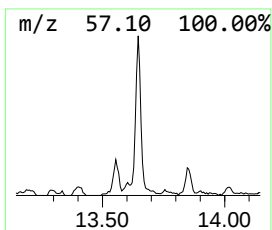
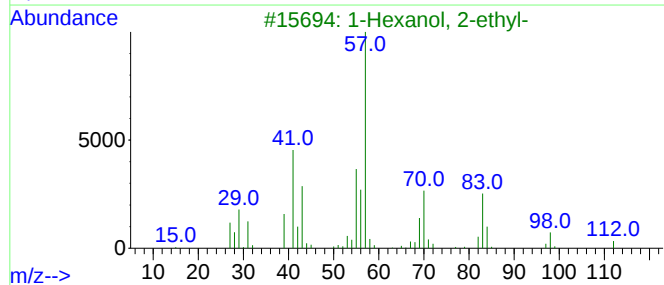
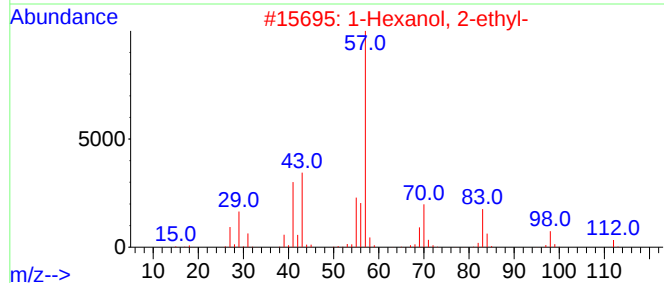
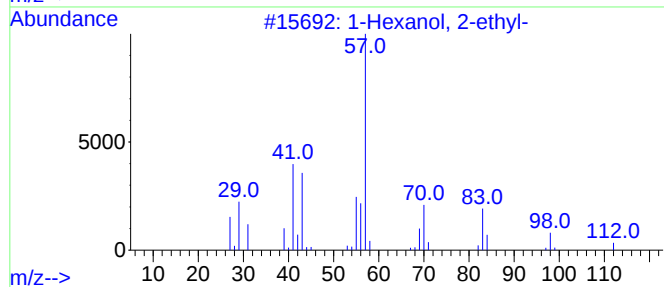
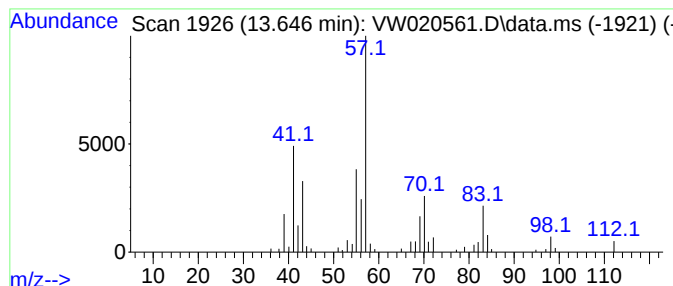
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM100821SMA.M
Quant Title : SFAM01.0

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.
13.646	1.85 ug/L	41571	1,4-Dichlorobenzene-d4	13.560

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	78
3		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
4		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
5		Oxirane, [[(2-ethylhexyl)oxy]met...	186	C11H22O2	002461-15-6	50



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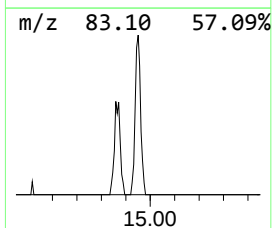
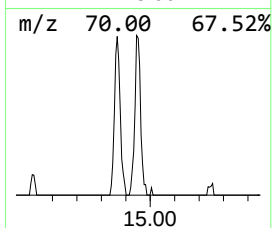
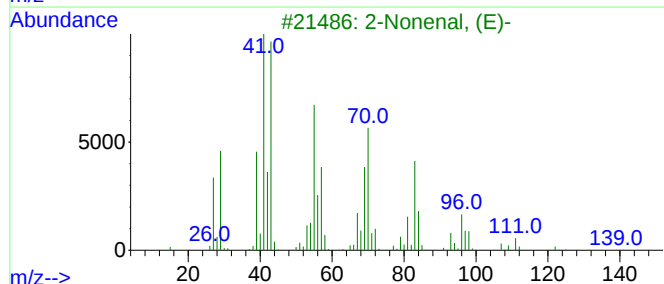
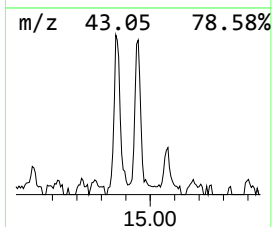
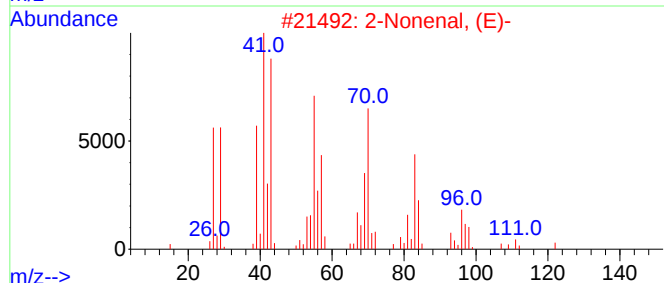
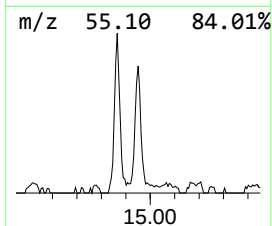
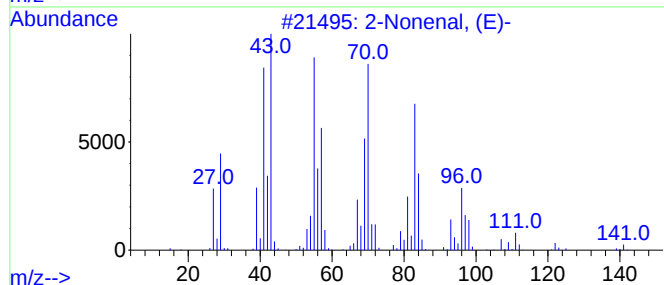
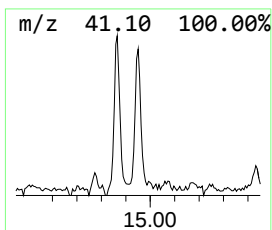
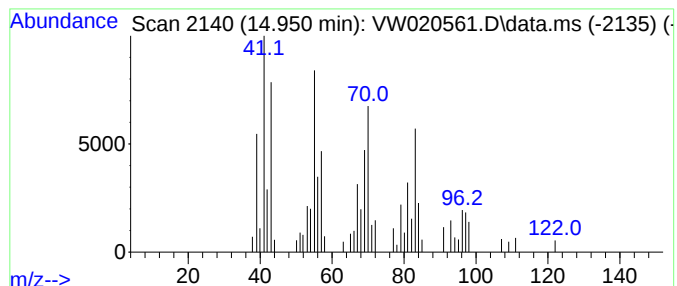
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Peak Number 3 2-Nonenal, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.950	1.26 ug/L	28241	1,4-Dichlorobenzene-d4	13.560

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonenal, (E)-			140	C9H16O	018829-56-6	64
2	2-Nonenal, (E)-			140	C9H16O	018829-56-6	64
3	2-Nonenal, (E)-			140	C9H16O	018829-56-6	58
4	1-Decanol			158	C10H22O	000112-30-1	47
5	2-Decenal, (Z)-			154	C10H18O	002497-25-8	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	13.646	1.9	ug/L	41571	3	13.560	561766	25.0
2-Nonenal, (E)-	14.950	1.3	ug/L	28241	3	13.560	561766	25.0