

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW031921\
 Data File : VW018407.D
 Acq On : 19 Mar 2021 23:39
 Operator : SY/VA
 Sample : M1685-08RE
 Misc : 5.54G/10ML/MSVOA_W/SOIL
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 BG494RE

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\SOM2WLM031921S.M

Title : VOC Analysis

Signal : TIC: VW018407.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.361	70	75	86	rVB	96008	199516	19.24%	2.862%
2	2.891	158	162	172	rVB	70595	165960	16.01%	2.381%
3	3.373	239	241	242	rBV	1135	924	0.09%	0.013%
4	3.854	318	320	322	rBV3	642	693	0.07%	0.010%
5	4.025	334	348	360	rBV2	117654	382857	36.93%	5.493%
6	4.232	380	382	384	rBV3	896	662	0.06%	0.009%
7	4.397	399	409	419	rBV2	12266	37051	3.57%	0.532%
8	4.525	429	430	436	rBV4	562	756	0.07%	0.011%
9	4.757	466	468	469	rBV	675	519	0.05%	0.007%
10	4.818	475	478	480	rBV3	629	719	0.07%	0.010%
11	4.921	485	495	507	rVV2	14857	53140	5.13%	0.762%
12	5.068	518	519	523	rVB3	705	633	0.06%	0.009%
13	5.110	523	526	529	rBV2	388	501	0.05%	0.007%
14	5.147	529	532	533	rBV2	700	817	0.08%	0.012%
15	5.281	552	554	559	rVB3	578	721	0.07%	0.010%
16	5.647	612	614	616	rBV3	541	501	0.05%	0.007%
17	5.683	618	620	623	rBV2	447	524	0.05%	0.008%
18	5.781	629	636	637	rBV6	3716	6271	0.60%	0.090%
19	5.860	647	649	653	rVB4	653	808	0.08%	0.012%
20	5.945	653	663	671	rBV3	5988	15862	1.53%	0.228%
21	6.055	679	681	683	rBV	406	368	0.04%	0.005%
22	6.104	688	689	693	rBV4	573	626	0.06%	0.009%
23	6.195	702	704	705	rBV	380	391	0.04%	0.006%
24	6.305	719	722	724	rBV2	403	500	0.05%	0.007%
25	6.366	731	732	735	rVB3	735	564	0.05%	0.008%
26	6.439	742	744	746	rBV2	487	556	0.05%	0.008%
27	6.464	746	748	751	rVB4	512	523	0.05%	0.008%
28	6.720	787	790	792	rBV3	670	589	0.06%	0.008%
29	6.823	804	807	809	rVB2	552	558	0.05%	0.008%
30	6.842	809	810	812	rBV2	480	456	0.04%	0.007%
31	6.903	812	820	822	rBV5	1920	4439	0.43%	0.064%
32	7.012	836	838	839	rBV	492	447	0.04%	0.006%
33	7.073	840	848	869	rVV3	43941	148873	14.36%	2.136%
34	7.384	897	899	902	rVB2	524	488	0.05%	0.007%
35	7.512	918	920	921	rBV2	525	366	0.04%	0.005%
36	7.646	930	942	953	rBV	179413	438859	42.33%	6.296%

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 Title : VOC Analysis

37	7.781	963	964	969	rVB4	948	1370	0.13%	0.020%
38	7.909	984	985	988	rBV3	776	612	0.06%	0.009%
39	8.030	1003	1005	1008	rVB3	487	529	0.05%	0.008%
40	8.067	1008	1011	1012	rBV2	534	548	0.05%	0.008%
41	8.140	1020	1023	1025	rBB3	482	495	0.05%	0.007%
42	8.177	1025	1029	1031	rBV2	559	655	0.06%	0.009%
43	8.274	1034	1045	1065	rBV2	342294	1036747	100.00%	14.874%
44	8.549	1084	1090	1091	rBV6	2957	4453	0.43%	0.064%
45	8.701	1111	1115	1116	rBV4	2097	2101	0.20%	0.030%
46	8.774	1126	1127	1130	rVB3	486	368	0.04%	0.005%
47	8.841	1130	1138	1148	rBV	359028	705743	68.07%	10.125%
48	9.042	1167	1171	1172	rBV3	1126	1221	0.12%	0.018%
49	9.171	1188	1192	1194	rBV2	730	871	0.08%	0.012%
50	9.274	1201	1209	1218	rBV	233182	474375	45.76%	6.806%
51	9.402	1227	1230	1242	rVB6	2589	6291	0.61%	0.090%
52	9.658	1268	1272	1280	rVB4	1872	3337	0.32%	0.048%
53	9.737	1283	1285	1287	rVB3	641	470	0.05%	0.007%
54	9.756	1287	1288	1290	rBV	460	365	0.04%	0.005%
55	9.926	1312	1316	1318	rBV4	923	1413	0.14%	0.020%
56	9.957	1318	1321	1324	rBV4	513	739	0.07%	0.011%
57	10.036	1327	1334	1342	rBV	98887	173842	16.77%	2.494%
58	10.189	1358	1359	1361	rBV	597	437	0.04%	0.006%
59	10.250	1367	1369	1370	rVB2	701	464	0.04%	0.007%
60	10.323	1370	1381	1389	rBV	428884	763381	73.63%	10.952%
61	10.579	1417	1423	1429	rBV	60093	104137	10.04%	1.494%
62	10.701	1438	1443	1451	rVB	19440	34010	3.28%	0.488%
63	10.865	1464	1470	1474	rBV	13591	23323	2.25%	0.335%
64	10.926	1474	1480	1494	rVB	157312	273106	26.34%	3.918%
65	11.073	1499	1504	1513	rVB6	9093	17644	1.70%	0.253%
66	11.231	1529	1530	1531	rBV	845	455	0.04%	0.007%
67	11.512	1572	1576	1577	rBV3	1263	1710	0.16%	0.025%
68	11.633	1588	1596	1604	rBV	382606	657444	63.41%	9.432%
69	12.261	1698	1699	1702	rVB2	910	635	0.06%	0.009%
70	12.292	1702	1704	1707	rBV3	545	766	0.07%	0.011%
71	12.341	1707	1712	1716	rVV5	4470	7973	0.77%	0.114%
72	12.402	1720	1722	1726	rVV4	700	845	0.08%	0.012%
73	12.469	1730	1733	1737	rVB4	1259	1345	0.13%	0.019%
74	12.499	1737	1738	1740	rVB2	688	462	0.04%	0.007%
75	12.542	1740	1745	1747	rBV3	622	994	0.10%	0.014%
76	12.603	1749	1755	1762	rBV	57821	95807	9.24%	1.375%

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Title : VOC Analysis

77	12.694	1762	1770	1778	rBV	192949	328944	31.73%	4.719%
78	12.853	1794	1796	1798	rBV3	766	483	0.05%	0.007%
79	12.883	1798	1801	1803	rBV3	581	698	0.07%	0.010%
80	12.932	1806	1809	1818	rVB7	2907	6322	0.61%	0.091%
81	13.048	1827	1828	1831	rBV3	763	404	0.04%	0.006%
82	13.292	1862	1868	1879	rVB6	5872	12584	1.21%	0.181%
83	13.395	1879	1885	1891	rBV6	5217	10785	1.04%	0.155%
84	13.456	1893	1895	1898	rBV3	740	993	0.10%	0.014%
85	13.560	1905	1912	1918	rBV	203505	338181	32.62%	4.852%
86	13.755	1941	1944	1948	rBV3	1954	3449	0.33%	0.049%
87	13.853	1953	1960	1967	rBV	184939	300928	29.03%	4.317%
88	14.017	1983	1987	1989	rBV4	1881	2220	0.21%	0.032%
89	14.066	1990	1995	2004	rVB	28585	48114	4.64%	0.690%
90	14.328	2031	2038	2046	rBV6	10667	20225	1.95%	0.290%
91	14.481	2060	2063	2064	rBV2	555	609	0.06%	0.009%
92	14.517	2067	2069	2076	rVB6	1867	2998	0.29%	0.043%
93	14.718	2099	2102	2107	rVB6	3975	6129	0.59%	0.088%
94	14.974	2143	2144	2145	rBV	1002	456	0.04%	0.007%
95	15.102	2163	2165	2167	rBV3	1248	1090	0.11%	0.016%
96	15.316	2198	2200	2202	rBV2	1057	638	0.06%	0.009%
97	15.486	2224	2228	2234	rBV2	4798	8595	0.83%	0.123%
98	15.688	2256	2261	2265	rBV6	2283	3978	0.38%	0.057%
99	16.480	2389	2391	2392	rBV	1645	1145	0.11%	0.016%
100	16.529	2397	2399	2400	rVB2	1158	510	0.05%	0.007%

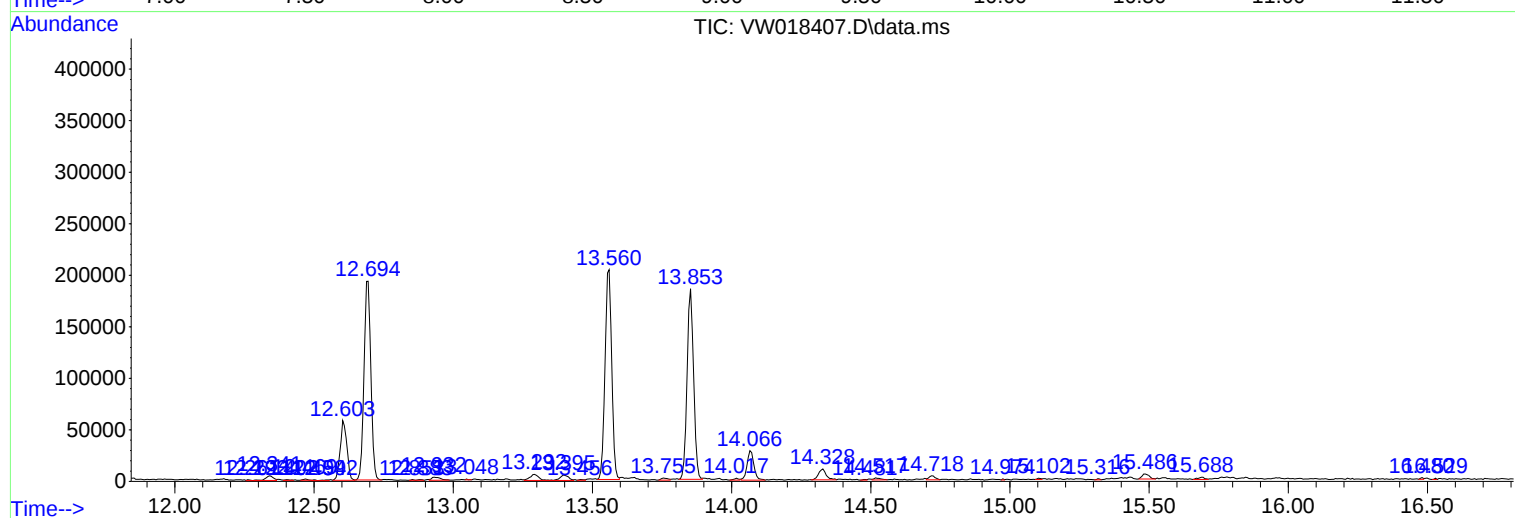
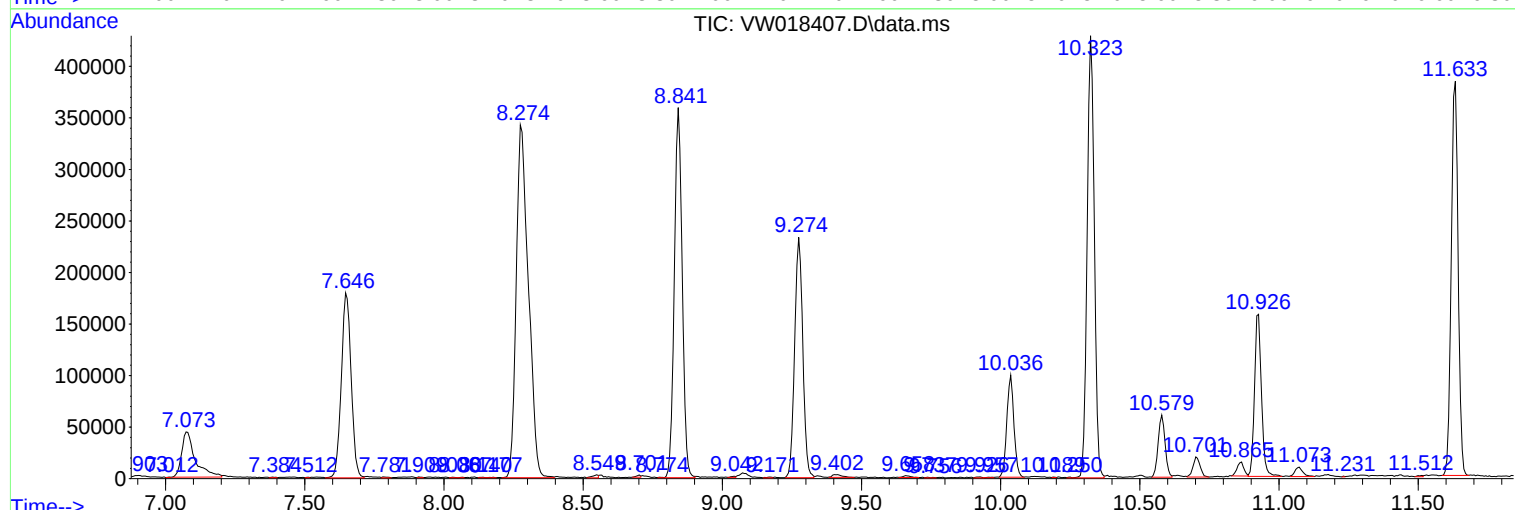
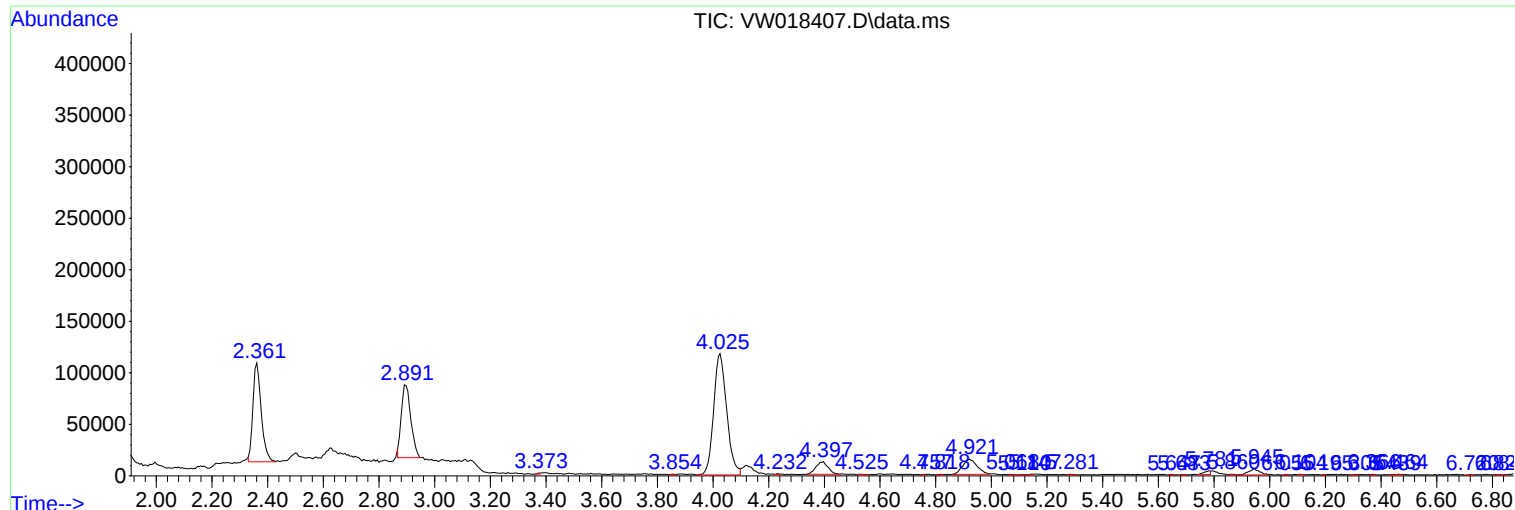
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SOM2WLM031921S.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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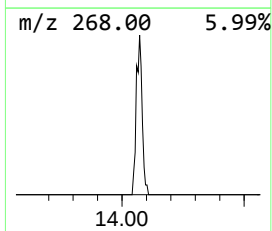
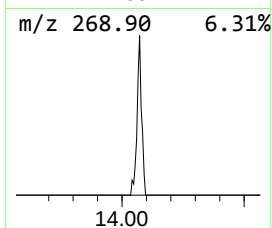
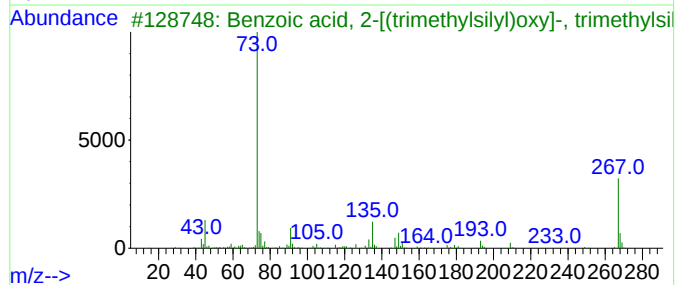
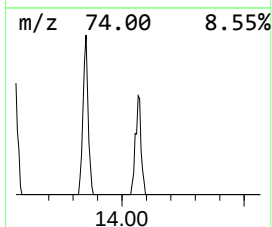
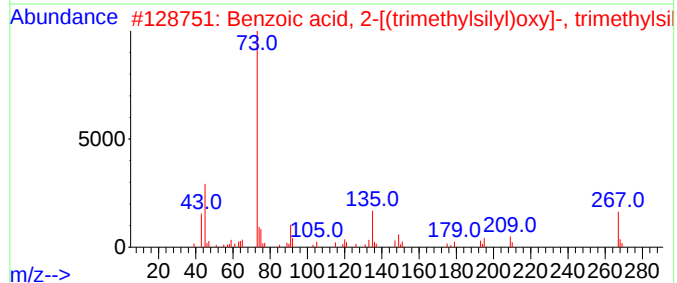
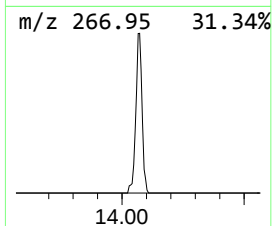
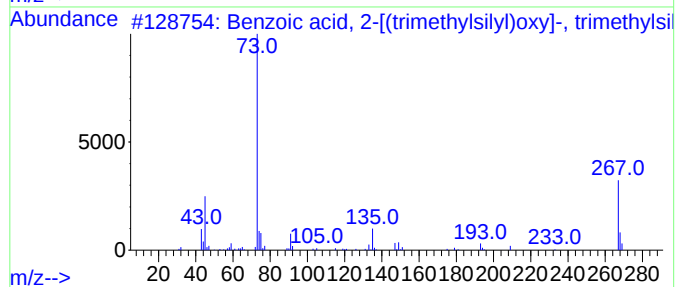
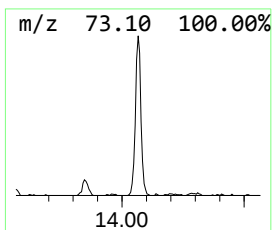
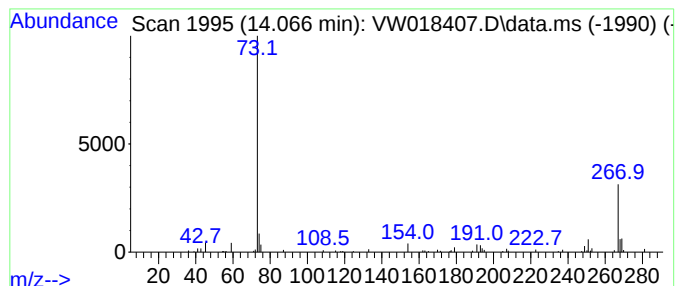
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SOM2WLM031921S.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzoic acid, 2-[(trimethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.066	3.56 ug/L	48114	1,4-Dichlorobenzene-d4	13.560

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-[(trimethylsilyl...]	282	C13H22O3Si2	003789-85-3	53
2			Benzoic acid, 2-[(trimethylsilyl...]	282	C13H22O3Si2	003789-85-3	38
3			Benzoic acid, 2-[(trimethylsilyl...]	282	C13H22O3Si2	003789-85-3	36
4			Benzoic acid, 2-[(trimethylsilyl...]	282	C13H22O3Si2	003789-85-3	36
5			Benzeneethanamine, N-[(pentaflu...]	475	C21H26F5NO2Si2	055429-85-1	33



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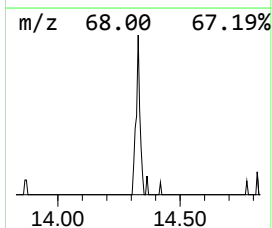
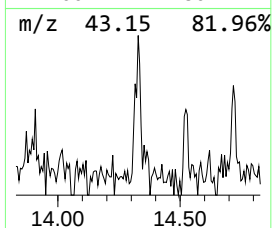
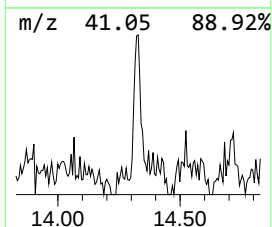
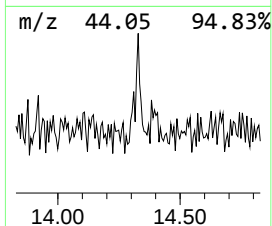
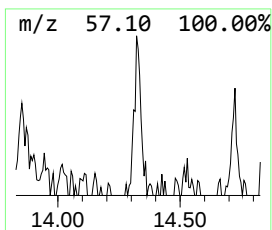
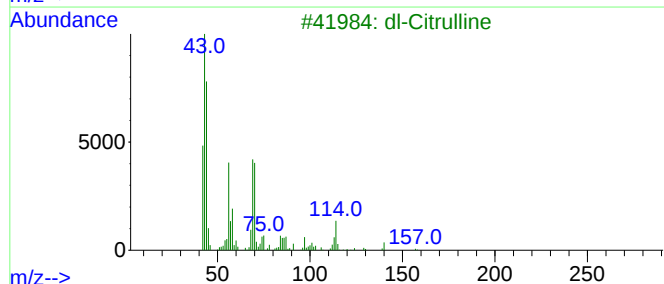
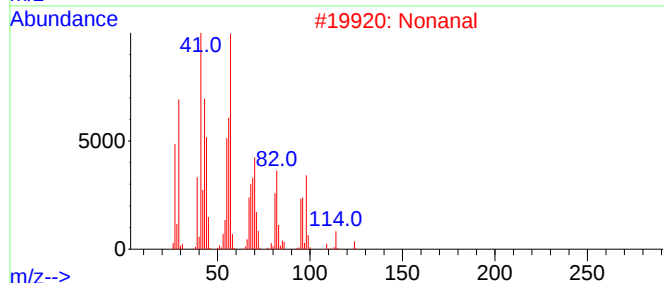
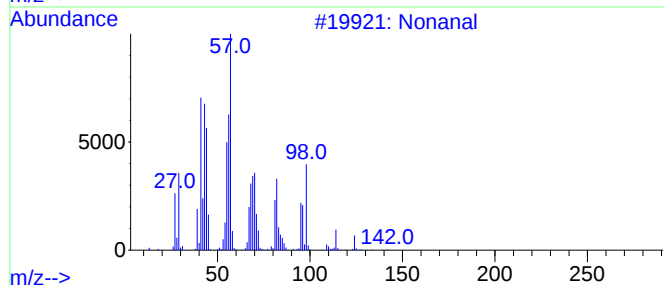
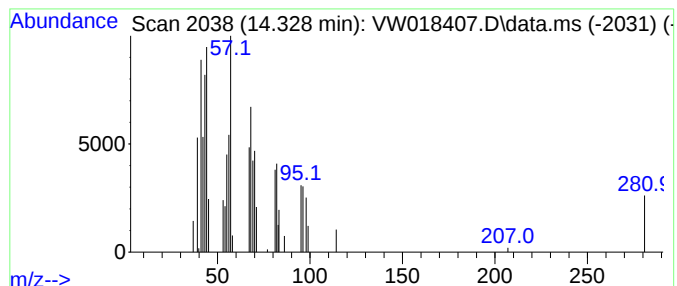
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Peak Number 5 Nonanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.328	1.50 ug/L	20225	1,4-Dichlorobenzene-d4	13.560

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	59
2			Nonanal	142	C9H18O	000124-19-6	38
3			dl-Citrulline	175	C6H13N3O3	000627-77-0	35
4			Oxacyclotetradecan-2-one, 13-met...	226	C14H26O2	057092-32-7	27
5			Tridecanal	198	C13H26O	010486-19-8	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzoic acid, 2...	14.066	3.6	ug/L	48114	3	13.560	338181	25.0
Nonanal	14.328	1.5	ug/L	20225	3	13.560	338181	25.0