

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD011922\
 Data File : VD071745.D
 Acq On : 19 Jan 2022 15:42
 Operator : VA/SY
 Sample : N1195-01
 Misc : 5.00G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 CL-02-011922

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % 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_D\Method\82D010722S.M
 Title : SW846 8260

Signal : TIC: VD071745.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.032	17	19	24	rBV	1400	1713	1.37%	0.186%
2	2.138	34	37	39	rVB3	1355	1429	1.14%	0.155%
3	2.226	43	52	54	rBV3	8499	21419	17.15%	2.326%
4	3.185	213	215	217	rVB	2480	1646	1.32%	0.179%
5	3.238	222	224	226	rVB	1695	1470	1.18%	0.160%
6	3.414	251	254	257	rVB	1332	1745	1.40%	0.190%
7	4.014	353	356	359	rVB2	1527	2125	1.70%	0.231%
8	4.202	385	388	392	rVB	1091	1810	1.45%	0.197%
9	4.526	441	443	444	rBV2	1653	1351	1.08%	0.147%
10	4.620	455	459	461	rBV2	1197	1731	1.39%	0.188%
11	4.661	464	466	469	rBV	1429	1524	1.22%	0.166%
12	4.697	471	472	476	rBV2	1008	1494	1.20%	0.162%
13	4.791	485	488	490	rBV2	1503	1919	1.54%	0.208%
14	4.908	507	508	513	rVB	1968	1829	1.46%	0.199%
15	4.949	513	515	517	rBV	1802	1579	1.26%	0.172%
16	5.155	545	550	552	rBV2	1626	2168	1.74%	0.235%
17	5.273	568	570	572	rBV2	1928	1386	1.11%	0.151%
18	5.402	587	592	595	rVB	1416	2580	2.07%	0.280%
19	5.479	602	605	608	rBV2	1361	1823	1.46%	0.198%
20	5.744	648	650	653	rBV2	1462	1967	1.58%	0.214%
21	5.808	658	661	663	rVV	1738	1545	1.24%	0.168%
22	6.438	766	768	771	rVB2	1582	1595	1.28%	0.173%
23	6.532	782	784	789	rBV2	1661	1757	1.41%	0.191%
24	6.938	850	853	855	rVB2	1593	1926	1.54%	0.209%
25	7.179	891	894	897	rBV2	2452	2241	1.79%	0.243%
26	7.267	907	909	911	rBV2	1655	1435	1.15%	0.156%
27	7.685	979	980	984	rBV2	1169	1335	1.07%	0.145%
28	7.826	1001	1004	1008	rBV2	1797	2507	2.01%	0.272%
29	7.914	1011	1019	1024	rVV3	17318	44446	35.60%	4.828%
30	7.979	1024	1030	1037	rVB2	30492	65972	52.84%	7.166%
31	8.173	1061	1063	1065	rBV	1557	1337	1.07%	0.145%
32	8.326	1080	1089	1097	rBV2	28982	68788	55.09%	7.471%
33	8.432	1105	1107	1112	rBV2	1150	1367	1.09%	0.148%
34	8.620	1136	1139	1141	rBV2	1363	1615	1.29%	0.175%
35	8.696	1151	1152	1155	rBV2	1616	1635	1.31%	0.178%
36	8.861	1172	1180	1189	rBV2	45791	91417	73.21%	9.929%

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37	8.996	1201	1203	1206	rBV2	1054	1336	1.07%	0.145%
38	9.355	1262	1264	1267	rVB2	1722	1575	1.26%	0.171%
39	9.402	1269	1272	1275	rBV2	1401	1749	1.40%	0.190%
40	9.673	1315	1318	1321	rBV2	806	1353	1.08%	0.147%

41	9.967	1364	1368	1369	rVB2	1386	1458	1.17%	0.158%
42	10.008	1371	1375	1376	rBV2	1407	1926	1.54%	0.209%
43	10.061	1378	1384	1385	rVB2	1742	2160	1.73%	0.235%
44	10.332	1423	1430	1438	rBV	67585	124863	100.00%	13.562%
45	10.396	1440	1441	1444	rVB2	1656	1537	1.23%	0.167%

46	10.455	1449	1451	1454	rVB	1810	1512	1.21%	0.164%
47	10.567	1466	1470	1473	rBV2	2495	2911	2.33%	0.316%
48	10.737	1494	1499	1502	rBV2	2043	2420	1.94%	0.263%
49	10.884	1522	1524	1525	rBV	1907	1460	1.17%	0.159%
50	10.931	1531	1532	1535	rBV	1837	1381	1.11%	0.150%

51	11.120	1563	1564	1566	rVB2	2337	1582	1.27%	0.172%
52	11.161	1569	1571	1574	rVB2	1088	1391	1.11%	0.151%
53	11.196	1574	1577	1580	rBV2	1468	2203	1.76%	0.239%
54	11.308	1594	1596	1600	rVB2	1444	1496	1.20%	0.162%
55	11.379	1606	1608	1611	rVB2	1824	1558	1.25%	0.169%

56	11.637	1645	1652	1659	rBV	66996	120120	96.20%	13.047%
57	11.702	1662	1663	1669	rVB2	1578	1845	1.48%	0.200%
58	11.755	1669	1672	1675	rBV2	1581	1558	1.25%	0.169%
59	11.937	1699	1703	1705	rVB2	1464	1816	1.45%	0.197%
60	11.967	1705	1708	1709	rBV2	2149	2525	2.02%	0.274%

61	12.131	1732	1736	1739	rVB2	1093	1555	1.25%	0.169%
62	12.237	1751	1754	1756	rBV3	1933	1740	1.39%	0.189%
63	12.555	1806	1808	1810	rVB2	1322	1348	1.08%	0.146%
64	12.620	1810	1819	1826	rBV3	51225	88508	70.88%	9.613%
65	12.896	1863	1866	1867	rVV	1543	1331	1.07%	0.145%

66	13.031	1887	1889	1891	rBV2	1196	1338	1.07%	0.145%
67	13.090	1897	1899	1902	rBV2	1408	1615	1.29%	0.175%
68	13.149	1907	1909	1912	rBV2	2181	2025	1.62%	0.220%
69	13.237	1921	1924	1929	rBV2	1460	2146	1.72%	0.233%
70	13.308	1934	1936	1937	rBV	2786	2075	1.66%	0.225%

71	13.508	1966	1970	1972	rBV2	1001	1419	1.14%	0.154%
72	13.561	1974	1979	1985	rVV	65938	108028	86.52%	11.734%
73	13.655	1990	1995	2002	rVV3	13729	20779	16.64%	2.257%
74	13.796	2017	2019	2022	rVB2	2163	2312	1.85%	0.251%
75	13.820	2022	2023	2026	rBV2	2220	1720	1.38%	0.187%

76	13.843	2026	2027	2031	rVB	1961	1501	1.20%	0.163%
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77	13.902	2036	2037	2040	rBV	1493	1543	1.24%	0.168%
78	14.002	2051	2054	2058	rVB3	1461	2115	1.69%	0.230%
79	14.043	2058	2061	2062	rBV	1507	1438	1.15%	0.156%
80	14.084	2067	2068	2071	rVB2	2013	2011	1.61%	0.218%
81	14.196	2086	2087	2090	rBV2	1808	1435	1.15%	0.156%
82	14.249	2093	2096	2098	rBV3	2096	2162	1.73%	0.235%
83	14.378	2117	2118	2121	rBV2	1564	1879	1.50%	0.204%
84	14.449	2128	2130	2134	rBV3	1720	2453	1.96%	0.266%
85	14.525	2140	2143	2147	rBV4	2422	2735	2.19%	0.297%
86	14.637	2159	2162	2164	rBV3	2073	2813	2.25%	0.306%
87	14.690	2169	2171	2173	rBV2	1534	1704	1.36%	0.185%
88	14.955	2214	2216	2218	rBV2	2101	1608	1.29%	0.175%
89	15.384	2288	2289	2292	rVB2	2250	1468	1.18%	0.159%
90	15.578	2320	2322	2325	rVB2	2887	2033	1.63%	0.221%
91	15.649	2332	2334	2339	rVB3	2065	2224	1.78%	0.242%
92	15.737	2348	2349	2352	rBV2	2585	2082	1.67%	0.226%
93	15.902	2375	2377	2380	rBV3	1298	1372	1.10%	0.149%
94	15.949	2383	2385	2387	rBV2	1758	1888	1.51%	0.205%
95	16.114	2411	2413	2416	rBV4	1825	1337	1.07%	0.145%
96	16.272	2438	2440	2443	rBV3	1729	2181	1.75%	0.237%
97	16.449	2464	2470	2474	rBV5	1934	4824	3.86%	0.524%
98	16.525	2481	2483	2487	rBV3	2453	3432	2.75%	0.373%
99	16.596	2494	2495	2499	rVB3	2329	2100	1.68%	0.228%
100	16.637	2499	2502	2505	rBV2	2104	3035	2.43%	0.330%

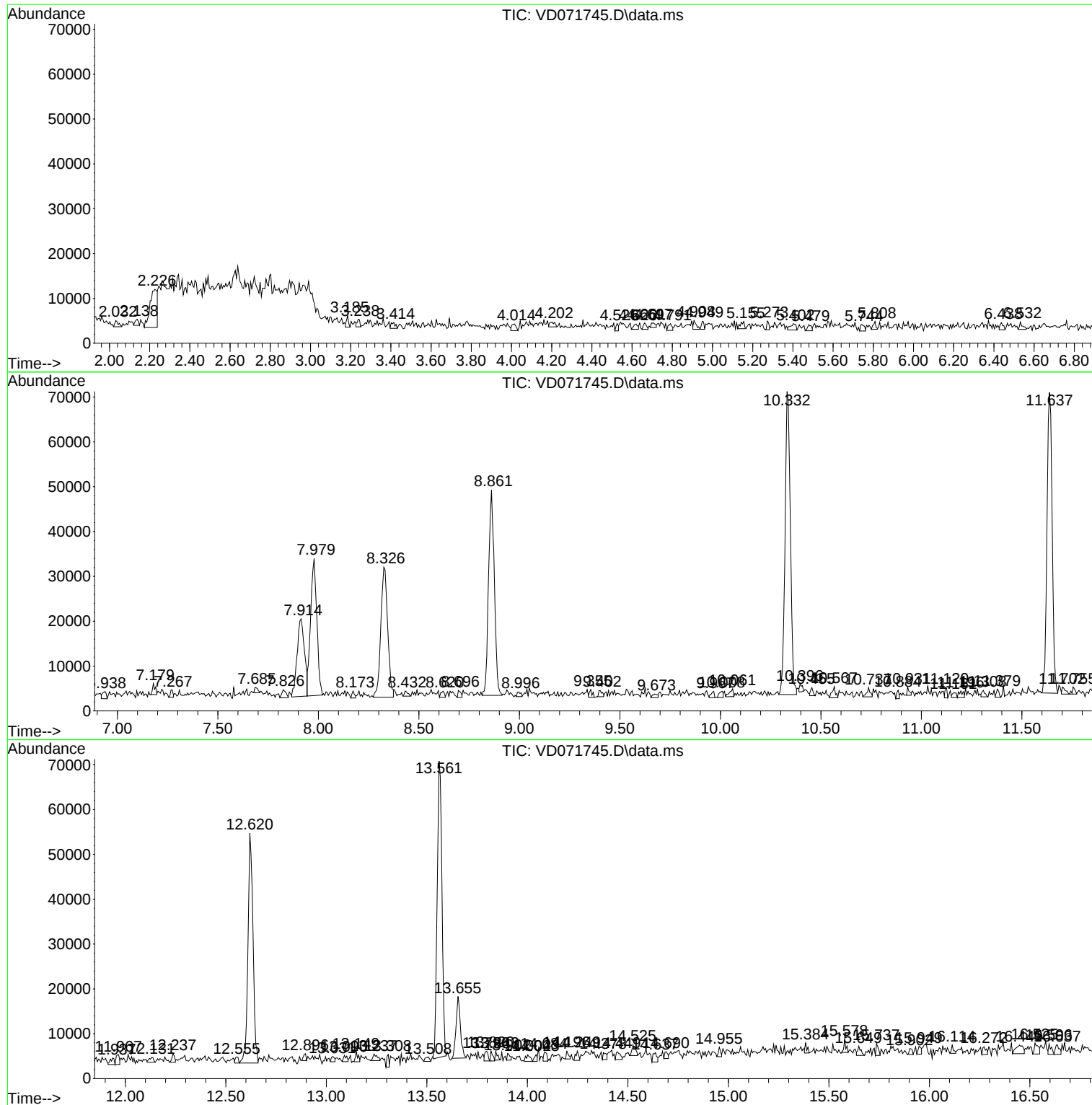
Sum of corrected areas: 920673

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D010722S.M
Quant Title : SW846 8260

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



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Instrument :
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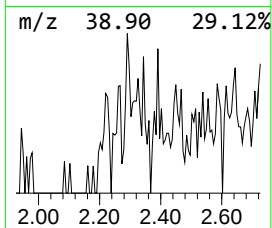
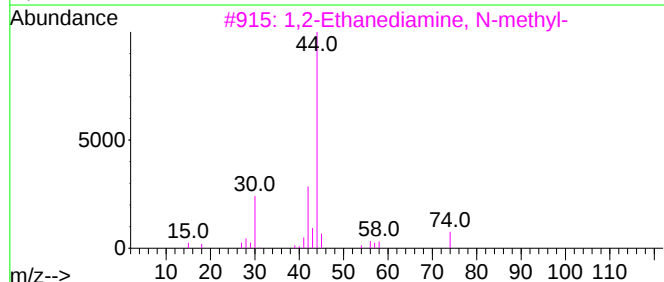
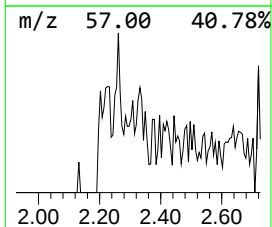
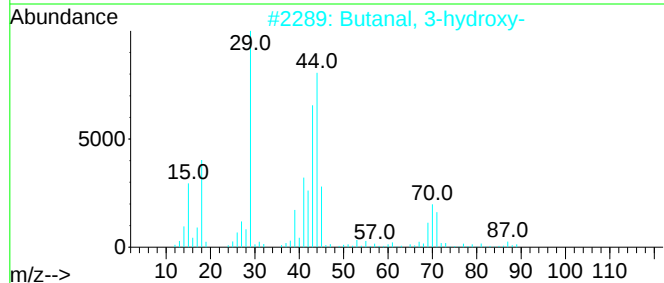
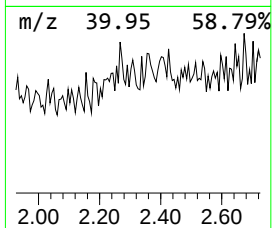
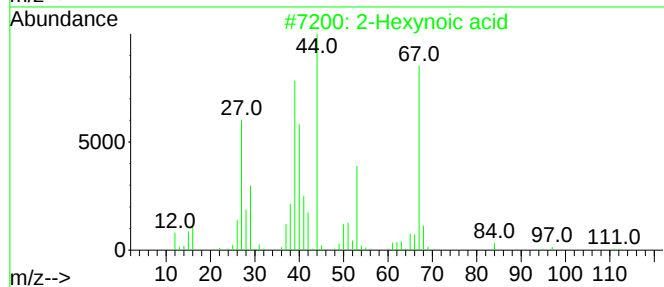
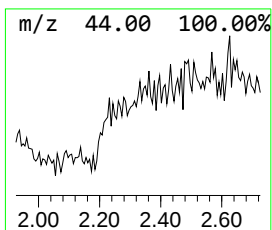
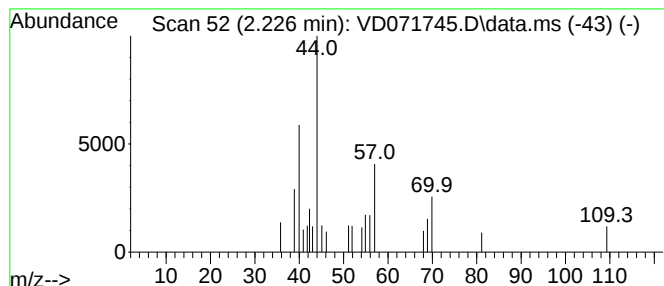
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D010722S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.226 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.226	16.23 ug/l	21419	Pentafluorobenzene	7.979

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexynoic acid			112	C6H8O2	000764-33-0	9
2	Butanal, 3-hydroxy-			88	C4H8O2	000107-89-1	9
3	1,2-Ethanediamine, N-methyl-			74	C3H10N2	000109-81-9	9
4	dL-Alanine			89	C3H7NO2	000302-72-7	9
5	1-Sec-butyl diaziridine			100	C5H12N2	033657-34-0	9



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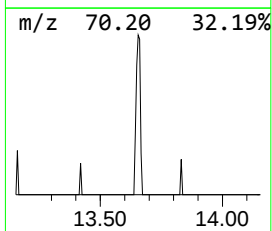
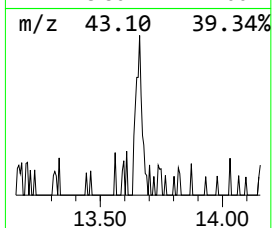
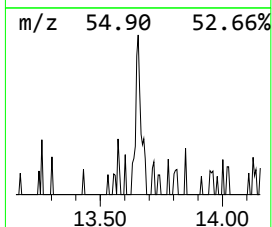
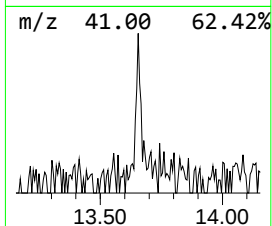
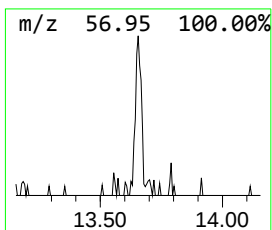
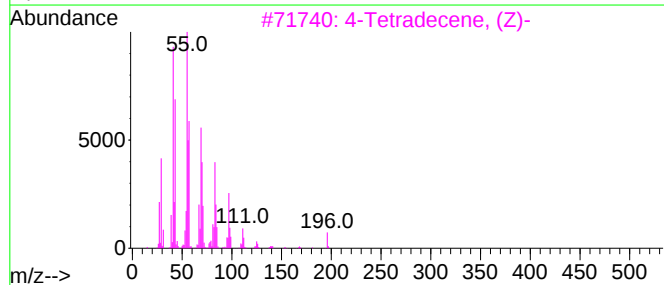
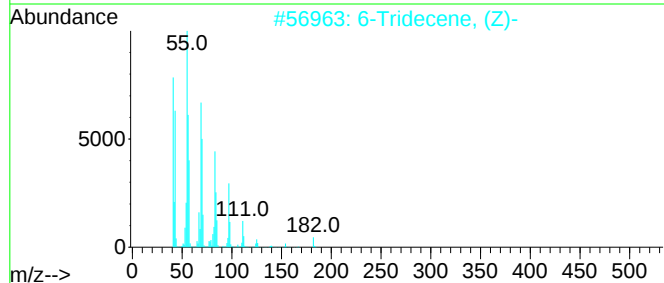
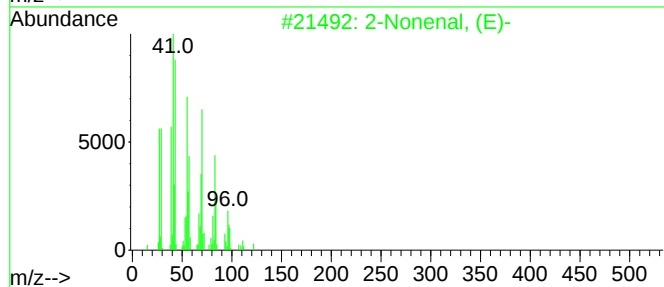
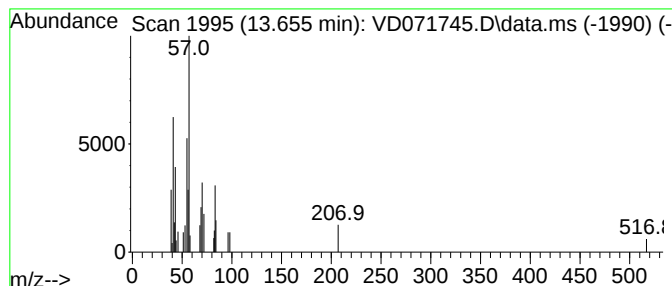
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D010722S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown13.655 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.655	9.62 ug/l	20779	1,4-Dichlorobenzene-d4		13.561

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonenal, (E)-		140	C9H16O	018829-56-6	47
2	6-Tridecene, (Z)-		182	C13H26	006508-77-6	38
3	4-Tetradecene, (Z)-		196	C14H28	041446-65-5	38
4	Bicyclo[3.1.0]hexan-2-ol		98	C6H10O	1000194-18-6	38
5	Formic acid, decyl ester		186	C11H22O2	005451-52-5	38



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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
unknown2.226	2.226	16.2	ug/l	21419	1	7.979	65972	50.0
unknown13.655	13.655	9.6	ug/l	20779	4	13.561	108028	50.0