

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD081023\
 Data File : VD076960.D
 Acq On : 10 Aug 2023 14:11
 Operator : JC/SY
 Sample : 03965-01
 Misc : 4.94G/10.0ml/MSVOA_D/SOIL
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 A4832

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_D\Method\SFAMDLM080323SMA.M

Title : SFAM01.0

Signal : TIC: VD076960.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.740	12	26	38	rBV	784587	1323033	100.00%	23.482%
2	2.146	92	95	96	rBV	2755	2695	0.20%	0.048%
3	2.269	111	116	127	rVB	119879	177378	13.41%	3.148%
4	2.799	199	206	214	rVB	96223	181635	13.73%	3.224%
5	3.293	287	290	293	rBV2	1881	2575	0.19%	0.046%
6	3.316	293	294	297	rVB2	1312	841	0.06%	0.015%
7	3.911	386	395	405	rBV	84294	220965	16.70%	3.922%
8	4.022	413	414	417	rVB	1527	1049	0.08%	0.019%
9	4.081	420	424	425	rBV2	1071	1120	0.08%	0.020%
10	4.793	536	545	546	rBV3	3430	6651	0.50%	0.118%
11	4.952	570	572	574	rVB	1002	730	0.06%	0.013%
12	5.181	610	611	614	rBV2	622	659	0.05%	0.012%
13	5.222	617	618	623	rBV2	400	663	0.05%	0.012%
14	5.381	641	645	646	rBV	728	765	0.06%	0.014%
15	5.769	709	711	712	rBV2	1070	808	0.06%	0.014%
16	5.816	718	719	722	rVV2	1119	1425	0.11%	0.025%
17	6.022	751	754	756	rBV2	753	1015	0.08%	0.018%
18	6.257	791	794	795	rBV2	694	654	0.05%	0.012%
19	6.416	819	821	824	rVV2	785	893	0.07%	0.016%
20	6.505	832	836	837	rVV	837	733	0.06%	0.013%
21	6.563	843	846	847	rBV	599	714	0.05%	0.013%
22	6.599	849	852	854	rBV2	581	741	0.06%	0.013%
23	6.740	875	876	879	rVB2	850	664	0.05%	0.012%
24	6.816	887	889	891	rBV3	1274	1313	0.10%	0.023%
25	6.905	903	904	907	rBV	775	849	0.06%	0.015%
26	6.981	910	917	926	rBV2	14670	45174	3.41%	0.802%
27	7.252	960	963	967	rBV	899	862	0.07%	0.015%
28	7.404	986	989	991	rBV2	753	797	0.06%	0.014%
29	7.563	1004	1016	1029	rBV2	118232	303775	22.96%	5.392%
30	7.663	1032	1033	1036	rBV2	890	994	0.08%	0.018%
31	7.734	1042	1045	1048	rVB2	750	780	0.06%	0.014%
32	7.840	1061	1063	1065	rBV2	769	711	0.05%	0.013%
33	7.963	1081	1084	1085	rBV2	755	766	0.06%	0.014%
34	8.099	1102	1107	1109	rBV2	1424	2145	0.16%	0.038%
35	8.199	1113	1124	1139	rBV3	230769	700478	52.94%	12.432%
36	8.293	1139	1140	1144	rBV3	928	968	0.07%	0.017%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM080323SMA.M
 Title : SFAM01.0

37	8.363	1150	1152	1154	rVB2	864	728	0.06%	0.013%
38	8.399	1154	1158	1160	rBV2	795	1181	0.09%	0.021%
39	8.634	1193	1198	1203	rBV3	2614	5419	0.41%	0.096%
40	8.775	1215	1222	1231	rVV2	118986	245944	18.59%	4.365%
41	9.010	1258	1262	1263	rBV	1244	1477	0.11%	0.026%
42	9.098	1272	1277	1278	rBV2	754	715	0.05%	0.013%
43	9.210	1288	1296	1305	rBV	155333	322840	24.40%	5.730%
44	9.681	1374	1376	1379	rVB2	688	769	0.06%	0.014%
45	9.775	1391	1392	1395	rBV2	818	878	0.07%	0.016%
46	9.981	1416	1427	1435	rBV	80869	150224	11.35%	2.666%
47	10.057	1438	1440	1442	rVV	631	712	0.05%	0.013%
48	10.075	1442	1443	1446	rVB	1335	701	0.05%	0.012%
49	10.269	1467	1476	1484	rBV	300049	539078	40.75%	9.568%
50	10.428	1498	1503	1504	rVB2	824	1074	0.08%	0.019%
51	10.451	1506	1507	1510	rVV	1029	955	0.07%	0.017%
52	10.528	1513	1520	1526	rVV	53772	94403	7.14%	1.675%
53	10.663	1539	1543	1549	rVB4	7134	12112	0.92%	0.215%
54	10.722	1551	1553	1555	rBV2	828	723	0.05%	0.013%
55	10.798	1563	1566	1568	rBV3	3560	3127	0.24%	0.055%
56	10.881	1573	1580	1590	rVV	67932	125117	9.46%	2.221%
57	11.040	1605	1607	1608	rBV	817	691	0.05%	0.012%
58	11.134	1618	1623	1628	rBV4	5116	8995	0.68%	0.160%
59	11.222	1637	1638	1641	rVB2	1071	812	0.06%	0.014%
60	11.287	1644	1649	1653	rVV2	932	1622	0.12%	0.029%
61	11.363	1658	1662	1668	rVB4	4109	6256	0.47%	0.111%
62	11.581	1691	1699	1708	rBV	179494	294925	22.29%	5.234%
63	11.675	1710	1715	1719	rVB2	2218	3381	0.26%	0.060%
64	11.869	1746	1748	1751	rBV	947	810	0.06%	0.014%
65	11.963	1761	1764	1765	rBV	723	778	0.06%	0.014%
66	12.063	1779	1781	1782	rBV	1145	790	0.06%	0.014%
67	12.287	1816	1819	1822	rBV2	1135	1253	0.09%	0.022%
68	12.310	1822	1823	1826	rVV	1395	1059	0.08%	0.019%
69	12.428	1839	1843	1844	rBV	730	929	0.07%	0.016%
70	12.581	1862	1869	1874	rVB4	8285	15084	1.14%	0.268%
71	12.651	1874	1881	1889	rVB2	119628	208269	15.74%	3.696%
72	12.710	1889	1891	1892	rBV2	1159	987	0.07%	0.018%
73	12.839	1911	1913	1914	rBV	909	859	0.06%	0.015%
74	12.851	1914	1915	1918	rVB	1452	939	0.07%	0.017%
75	12.881	1918	1920	1921	rBV	1011	880	0.07%	0.016%
76	12.898	1921	1923	1926	rVV3	1492	1613	0.12%	0.029%

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Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM080323SMA.M
 Title : SFAM01.0

77	12.998	1938	1940	1945	rVB4	1814	2336	0.18%	0.041%
78	13.039	1945	1947	1952	rVB5	2263	2916	0.22%	0.052%
79	13.163	1963	1968	1973	rVB4	5397	9286	0.70%	0.165%
80	13.269	1982	1986	1990	rBV2	2105	2624	0.20%	0.047%
81	13.375	1998	2004	2010	rVB4	9191	14288	1.08%	0.254%
82	13.475	2017	2021	2022	rBV2	5116	6454	0.49%	0.115%
83	13.516	2023	2028	2034	rVV	126361	206853	15.63%	3.671%
84	13.728	2060	2064	2068	rBV3	8586	15780	1.19%	0.280%
85	13.816	2073	2079	2086	rVV2	180537	292322	22.09%	5.188%
86	13.869	2086	2088	2093	rVB5	4856	5945	0.45%	0.106%
87	14.045	2113	2118	2130	rVV6	3296	10084	0.76%	0.179%
88	14.422	2178	2182	2185	rBV3	1344	1638	0.12%	0.029%
89	14.469	2187	2190	2191	rBV2	2050	2353	0.18%	0.042%
90	14.481	2191	2192	2194	rVB2	2366	1176	0.09%	0.021%
91	14.604	2211	2213	2214	rBV2	1474	753	0.06%	0.013%
92	14.669	2218	2224	2225	rBV3	2173	3238	0.24%	0.057%
93	15.257	2322	2324	2327	rVB2	1727	1589	0.12%	0.028%
94	15.381	2344	2345	2349	rVB3	1598	1478	0.11%	0.026%
95	15.563	2375	2376	2379	rBV2	994	895	0.07%	0.016%
96	15.622	2384	2386	2389	rVV2	1207	958	0.07%	0.017%
97	15.904	2433	2434	2437	rBV2	1384	1112	0.08%	0.020%
98	16.069	2460	2462	2464	rBV3	1149	866	0.07%	0.015%
99	16.098	2464	2467	2468	rBV2	1753	1498	0.11%	0.027%
100	16.704	2569	2570	2571	rBV	1663	756	0.06%	0.013%

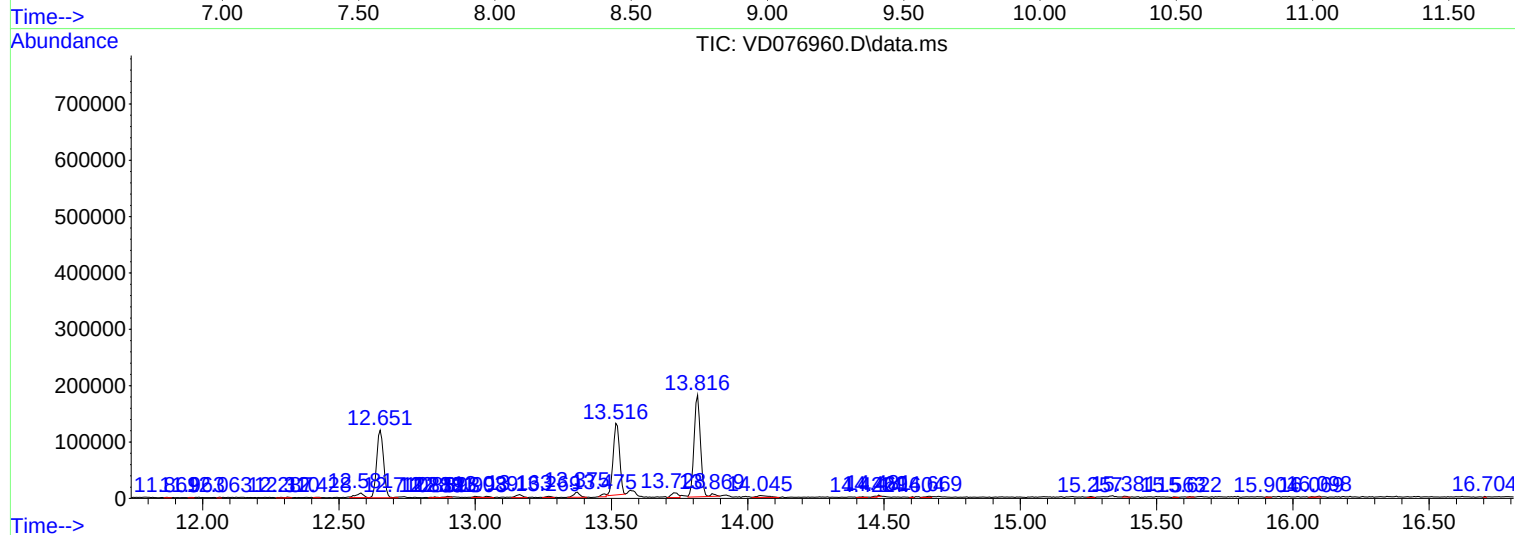
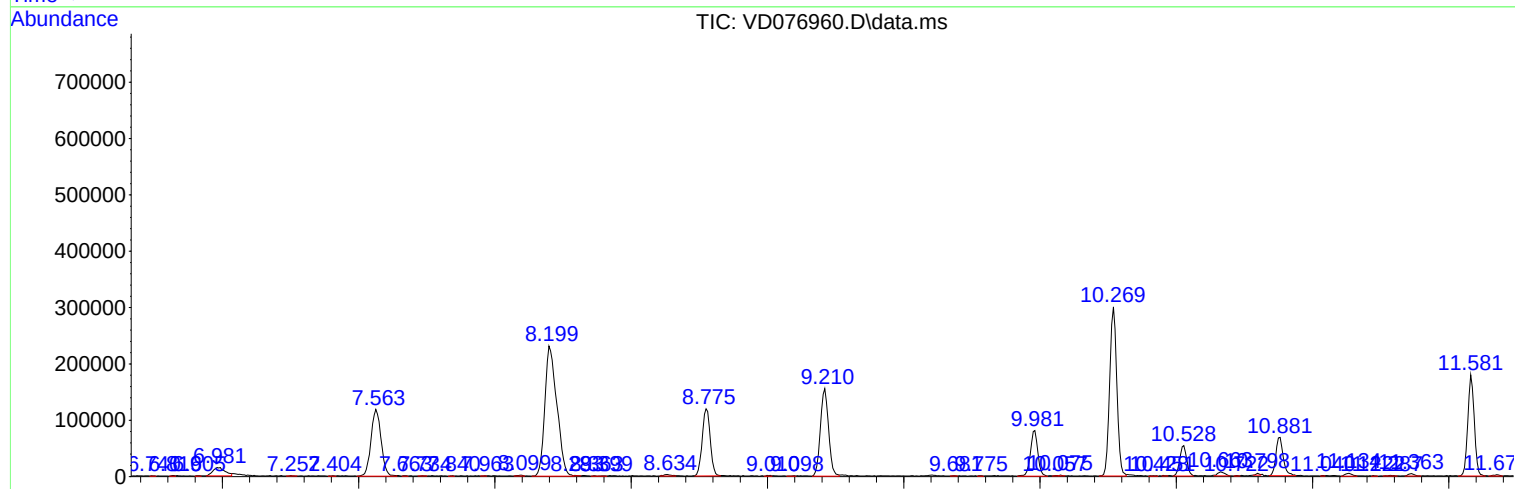
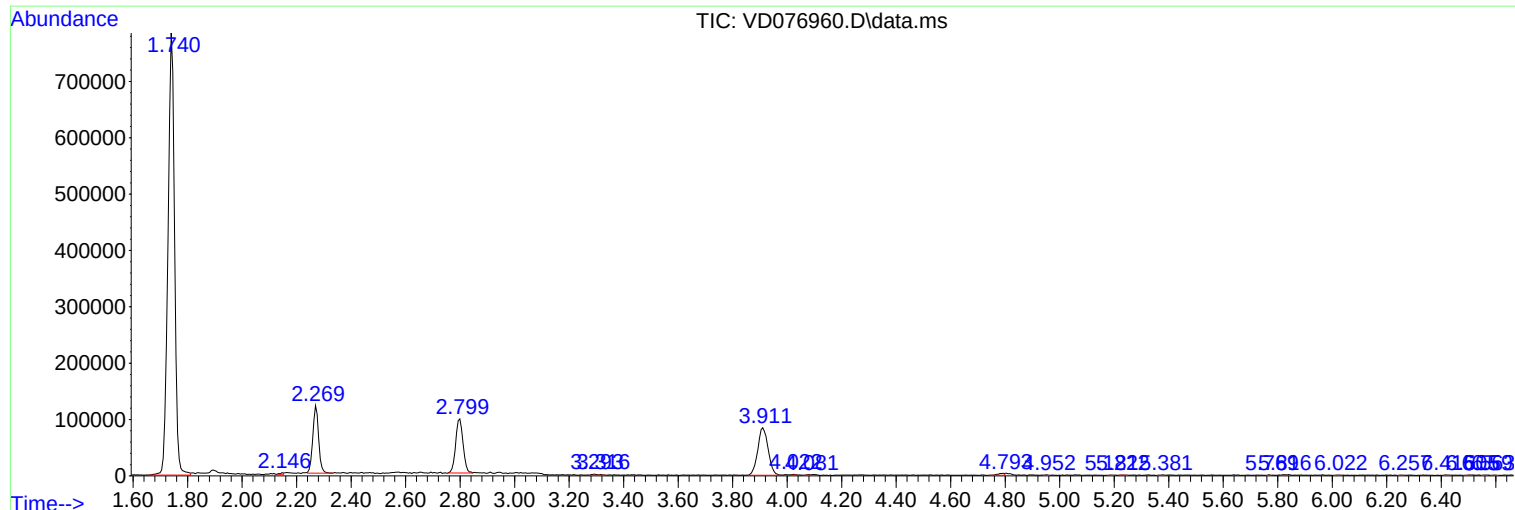
Sum of corrected areas: 5634325

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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_D
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM080323SMA.M
Quant Title : SFAM01.0

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



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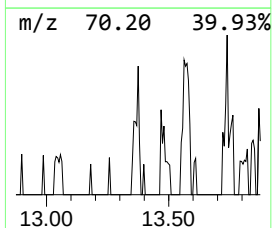
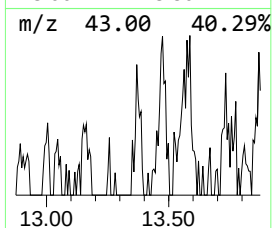
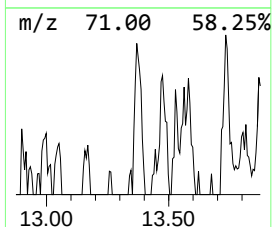
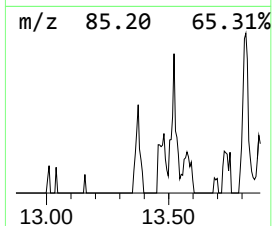
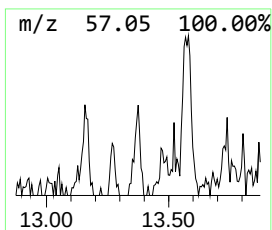
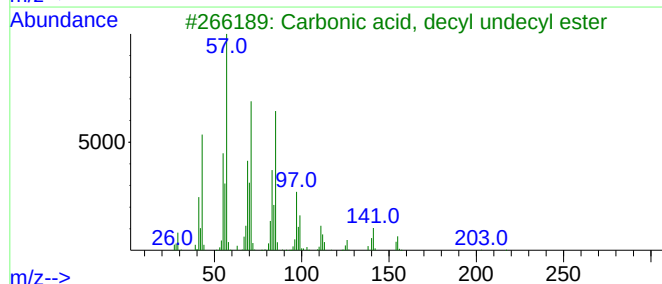
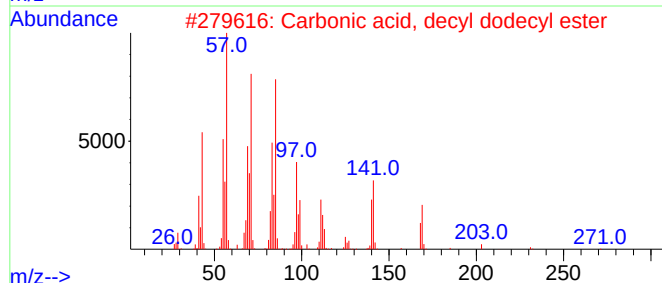
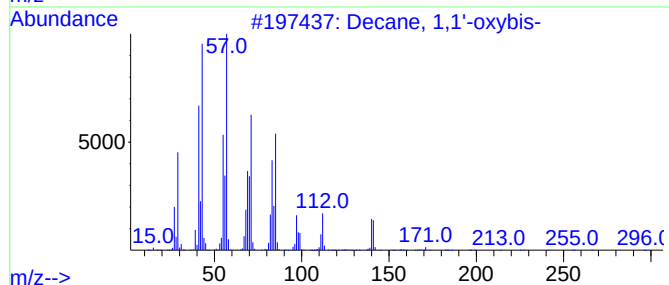
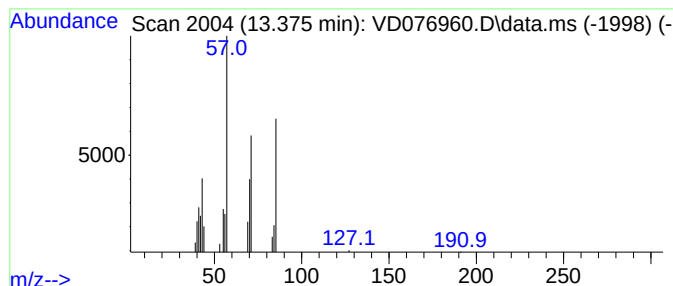
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM080323SMA.M
Quant Title : SFAM01.0

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

Peak Number 4 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.375	1.73 ug/L	14288	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 1,1'-oxybis-	298	C20H42O	002456-28-2	45
2			Carbonic acid, decyl dodecyl ester	370	C23H46O3	1000383-16-1	40
3			Carbonic acid, decyl undecyl ester	356	C22H44O3	1000383-16-0	40
4			Carbonic acid, decyl tridecyl ester	384	C24H48O3	1000383-16-2	40
5			Oxalic acid, 2-ethylhexyl isohex...	286	C16H30O4	1000309-38-8	40



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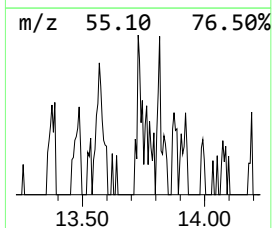
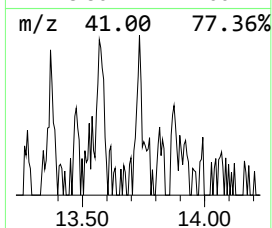
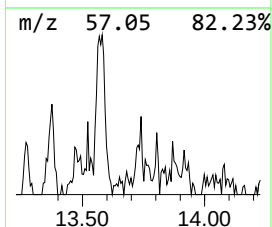
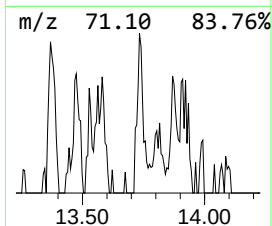
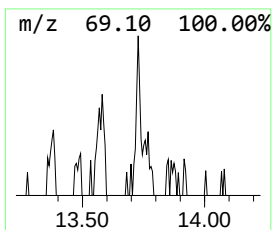
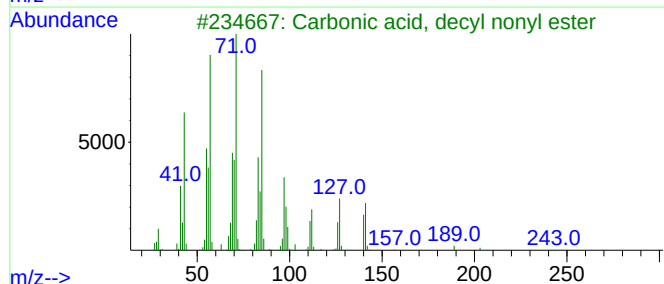
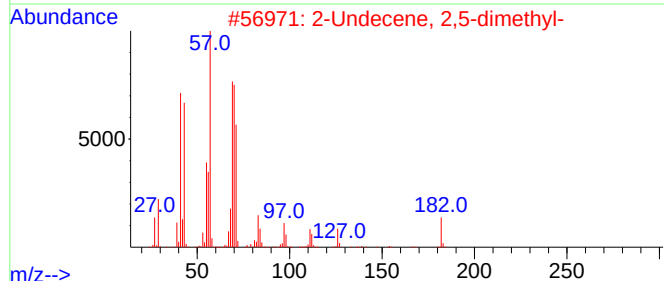
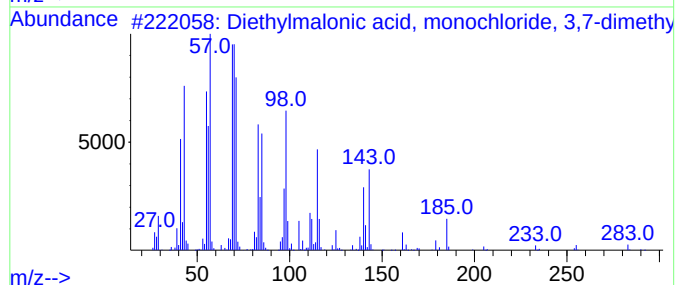
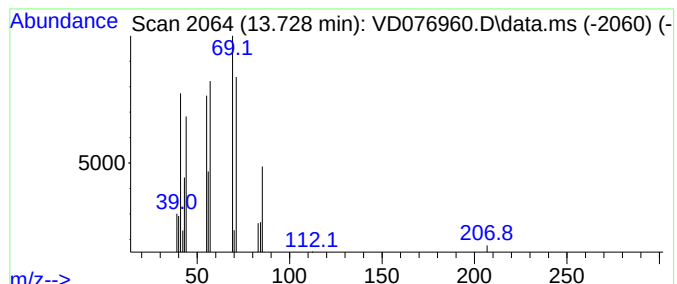
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\SFAMDLM080323SMA.M
Quant Title : SFAM01.0

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

Peak Number 5 Diethylmalonic acid, monochlorid... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.728	1.91 ug/L	15780	1,4-Dichlorobenzene-d4	13.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylmalonic acid, monochlorid...	318	C17H31ClO3	1000369-41-8	59
2			2-Undecene, 2,5-dimethyl-	182	C13H26	049622-16-4	50
3			Carbonic acid, decyl nonyl ester	328	C20H40O3	1000383-15-8	43
4			Carbonic acid, prop-1-en-2-yl te...	298	C18H34O3	1000382-90-9	38
5			5-Undecene, 4-methyl-	168	C12H24	143185-91-5	38



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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
unknown-01	13.375	1.7	ug/L	14288	3	13.516	206853	25.0
Diethylmalonic ...	13.728	1.9	ug/L	15780	3	13.516	206853	25.0