

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW031723\
 Data File : VW025410.D
 Acq On : 17 Mar 2023 11:16
 Operator : SY/MD
 Sample : 01927-11
 Misc : 6.25g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 DCAQ8

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\SFAMWLM030623SMA.M
 Title : SFAM01.0

Signal : TIC: VW025410.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	72	78	93	rVB	139555	343903	9.25%	1.337%
2	2.899	159	166	180	rVB2	132668	354250	9.53%	1.377%
3	3.289	226	230	232	rBV5	1675	2370	0.06%	0.009%
4	3.393	239	247	256	rBV2	21933	55763	1.50%	0.217%
5	3.460	256	258	262	rBV5	1669	1977	0.05%	0.008%
6	3.637	286	287	290	rVB3	2508	2128	0.06%	0.008%
7	3.667	290	292	294	rBV3	2541	2835	0.08%	0.011%
8	3.698	294	297	300	rVV5	3040	4905	0.13%	0.019%
9	3.728	300	302	304	rVV3	3716	4509	0.12%	0.018%
10	3.777	308	310	316	rVB7	2128	3377	0.09%	0.013%
11	3.826	316	318	320	rBV2	2238	2086	0.06%	0.008%
12	4.021	339	350	360	rBV2	369322	1149446	30.91%	4.467%
13	4.118	360	366	375	rVV	263041	736212	19.80%	2.861%
14	4.210	375	381	395	rVB2	67242	187578	5.04%	0.729%
15	4.399	405	412	421	rVB2	9287	27794	0.75%	0.108%
16	4.746	466	469	471	rVB4	1864	1959	0.05%	0.008%
17	4.856	483	487	488	rBV4	1835	2149	0.06%	0.008%
18	4.923	488	498	503	rBV3	15182	49315	1.33%	0.192%
19	5.069	518	522	525	rBV6	2332	4228	0.11%	0.016%
20	5.204	540	544	547	rBV5	1826	2988	0.08%	0.012%
21	5.710	623	627	630	rVB6	1932	3234	0.09%	0.013%
22	5.752	630	634	635	rBV3	2965	2701	0.07%	0.010%
23	5.825	644	646	651	rVB6	2561	2944	0.08%	0.011%
24	5.941	655	665	676	rBV2	20284	65081	1.75%	0.253%
25	6.234	710	713	716	rBV4	2246	2788	0.07%	0.011%
26	6.289	721	722	725	rVV3	2532	3021	0.08%	0.012%
27	6.344	728	731	733	rVB4	2251	2089	0.06%	0.008%
28	6.539	759	763	764	rBV4	2187	2788	0.07%	0.011%
29	6.594	769	772	774	rBV4	2124	2168	0.06%	0.008%
30	6.758	796	799	802	rBV5	1575	1907	0.05%	0.007%
31	6.972	829	834	836	rBV5	3971	5910	0.16%	0.023%
32	7.075	843	851	861	rBV	89264	266164	7.16%	1.034%
33	7.337	892	894	897	rVB4	1907	1908	0.05%	0.007%
34	7.648	934	945	958	rBV	613567	1494614	40.19%	5.809%
35	7.910	985	988	990	rBV4	1670	1956	0.05%	0.008%
36	7.971	995	998	1002	rVV6	1488	2140	0.06%	0.008%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM030623SMA.M
 Title : SFAM01.0

37	8.051	1008	1011	1014	rBV5	1561	2295	0.06%	0.009%
38	8.154	1024	1028	1030	rBV5	2551	3182	0.09%	0.012%
39	8.276	1038	1048	1068	rVV2	1286642	3718545	100.00%	14.451%
40	8.410	1068	1070	1075	rVB6	2276	2504	0.07%	0.010%
41	8.520	1085	1088	1089	rVV3	2212	2251	0.06%	0.009%
42	8.551	1090	1093	1096	rVB5	2785	3960	0.11%	0.015%
43	8.636	1104	1107	1108	rBV3	1926	2064	0.06%	0.008%
44	8.703	1110	1118	1127	rVB2	10014	25967	0.70%	0.101%
45	8.843	1131	1141	1154	rBV	1348371	2643426	71.09%	10.273%
46	9.014	1167	1169	1171	rBV2	1661	2052	0.06%	0.008%
47	9.154	1188	1192	1198	rVB8	3593	6595	0.18%	0.026%
48	9.276	1203	1212	1222	rBV	855654	1752288	47.12%	6.810%
49	9.630	1264	1270	1271	rBV6	2287	3762	0.10%	0.015%
50	9.770	1292	1293	1297	rBV4	2074	2253	0.06%	0.009%
51	9.928	1316	1319	1321	rVV4	2244	2373	0.06%	0.009%
52	10.032	1329	1336	1347	rVV	413042	759386	20.42%	2.951%
53	10.130	1347	1352	1361	rVV2	19938	39377	1.06%	0.153%
54	10.203	1361	1364	1368	rVB6	2378	3281	0.09%	0.013%
55	10.325	1373	1384	1392	rBV	1751708	3126488	84.08%	12.151%
56	10.514	1410	1415	1419	rVV8	7190	16721	0.45%	0.065%
57	10.575	1419	1425	1437	rVB	256902	451601	12.14%	1.755%
58	10.703	1442	1446	1452	rVB6	5644	9819	0.26%	0.038%
59	10.922	1475	1482	1498	rVV	327532	570109	15.33%	2.216%
60	11.391	1555	1559	1560	rBV4	1621	1977	0.05%	0.008%
61	11.629	1591	1598	1606	rBV	1686222	2729687	73.41%	10.608%
62	11.830	1627	1631	1636	rVV6	6211	11775	0.32%	0.046%
63	11.952	1648	1651	1652	rBV3	2209	2427	0.07%	0.009%
64	11.971	1652	1654	1659	rVV6	2557	4275	0.11%	0.017%
65	12.032	1659	1664	1669	rVV9	5842	11616	0.31%	0.045%
66	12.135	1678	1681	1683	rBV3	2335	3206	0.09%	0.012%
67	12.178	1683	1688	1696	rVV3	14784	31527	0.85%	0.123%
68	12.464	1731	1735	1738	rVV5	2550	3265	0.09%	0.013%
69	12.513	1741	1743	1746	rBV3	2397	2470	0.07%	0.010%
70	12.568	1748	1752	1754	rBV5	3015	3682	0.10%	0.014%
71	12.611	1756	1759	1763	rVB6	3891	4758	0.13%	0.018%
72	12.690	1765	1772	1782	rBV	525478	860594	23.14%	3.345%
73	12.830	1791	1795	1802	rVB9	5276	8361	0.22%	0.032%
74	12.928	1808	1811	1815	rBV5	3868	6742	0.18%	0.026%
75	13.019	1823	1826	1827	rBV3	2377	2042	0.05%	0.008%
76	13.105	1837	1840	1842	rBV4	2104	2210	0.06%	0.009%

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 Title : SFAM01.0

77	13.153	1844	1848	1852	rVV5	10434	17777	0.48%	0.069%
78	13.208	1852	1857	1867	rVV	78297	140888	3.79%	0.548%
79	13.287	1867	1870	1879	rVB9	9398	16942	0.46%	0.066%
80	13.470	1896	1900	1907	rBV9	6207	12842	0.35%	0.050%
81	13.556	1907	1914	1925	rVV	1317285	2081385	55.97%	8.089%
82	13.769	1946	1949	1952	rBV5	3211	3869	0.10%	0.015%
83	13.848	1954	1962	1970	rBV	1065547	1721630	46.30%	6.691%
84	14.062	1994	1997	1999	rBV3	4410	5926	0.16%	0.023%
85	14.147	2008	2011	2017	rBV8	2751	4545	0.12%	0.018%
86	14.220	2017	2023	2024	rBV6	3731	4652	0.13%	0.018%
87	14.318	2032	2039	2047	rBV6	4930	16189	0.44%	0.063%
88	14.519	2066	2072	2076	rBV9	1885	3394	0.09%	0.013%
89	14.617	2086	2088	2097	rVB10	4119	8546	0.23%	0.033%
90	14.720	2101	2105	2108	rBV6	1937	3378	0.09%	0.013%
91	14.781	2111	2115	2121	rBV9	3750	6460	0.17%	0.025%
92	14.927	2136	2139	2142	rBV4	2084	2378	0.06%	0.009%
93	15.123	2166	2171	2173	rBV6	2868	5738	0.15%	0.022%
94	15.366	2207	2211	2217	rVB9	3037	6473	0.17%	0.025%
95	15.470	2226	2228	2230	rBV3	2868	3230	0.09%	0.013%
96	15.543	2236	2240	2242	rBV5	3349	4889	0.13%	0.019%
97	15.781	2277	2279	2284	rBV7	1217	1914	0.05%	0.007%
98	16.171	2341	2343	2346	rVB4	2954	3006	0.08%	0.012%
99	16.299	2358	2364	2371	rBV4	5249	10037	0.27%	0.039%
100	16.458	2385	2390	2391	rBV5	1921	3102	0.08%	0.012%

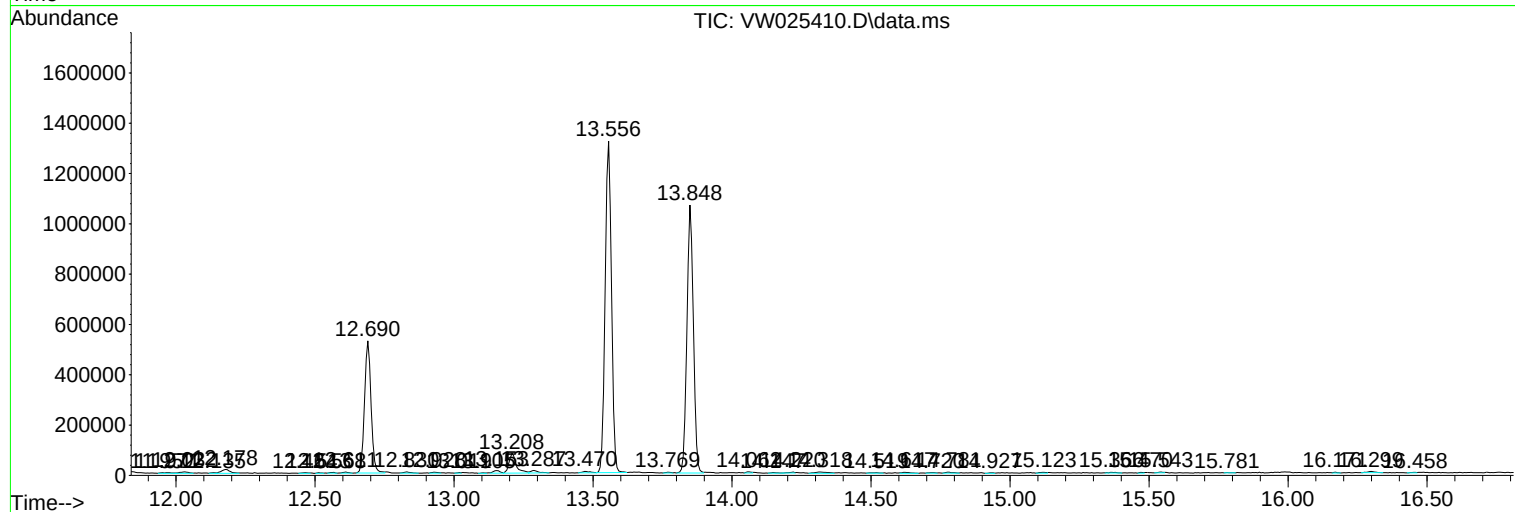
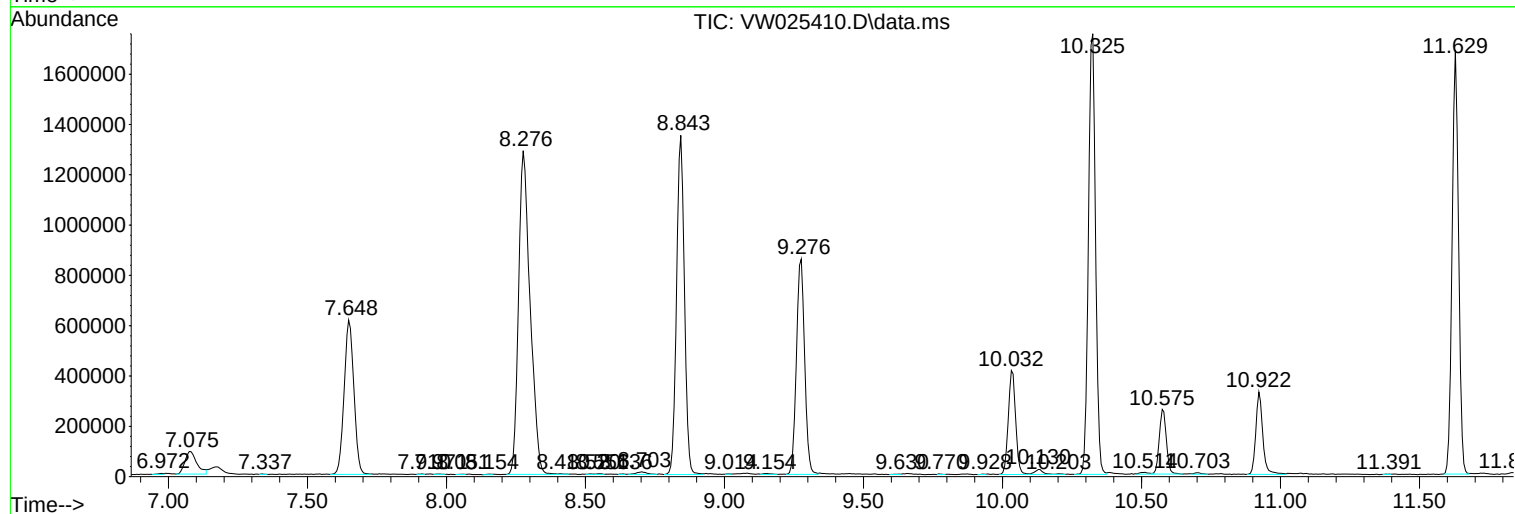
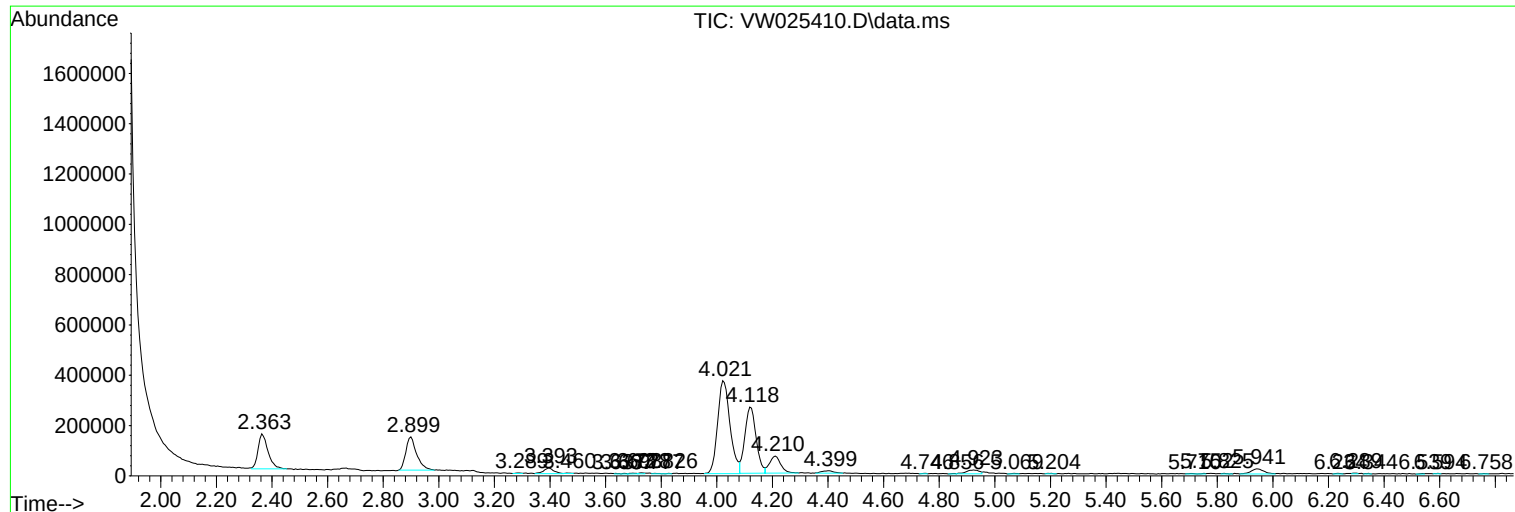
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM030623SMA.M
Quant Title : SFAM01.0

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



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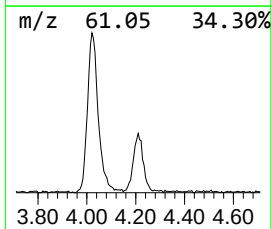
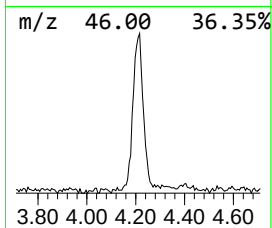
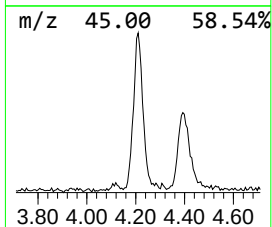
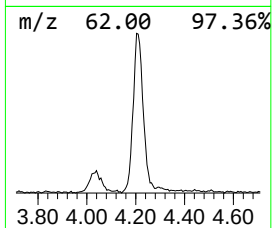
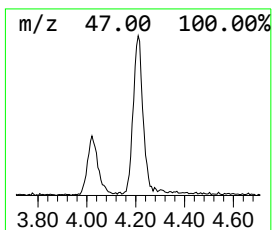
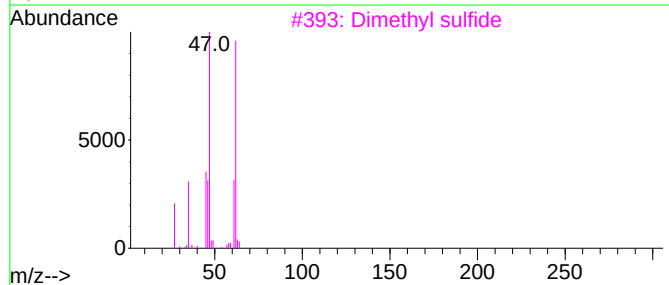
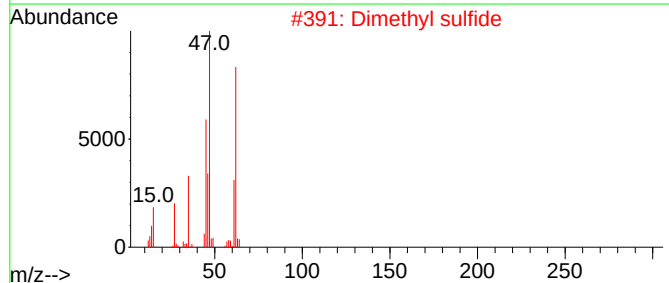
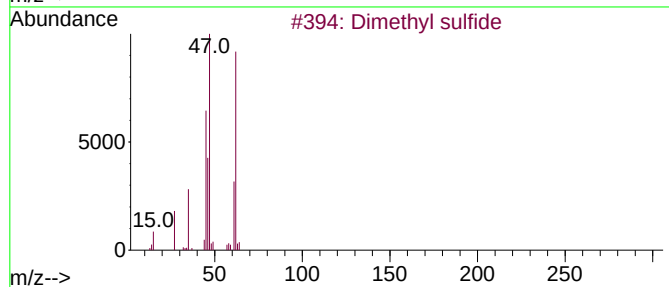
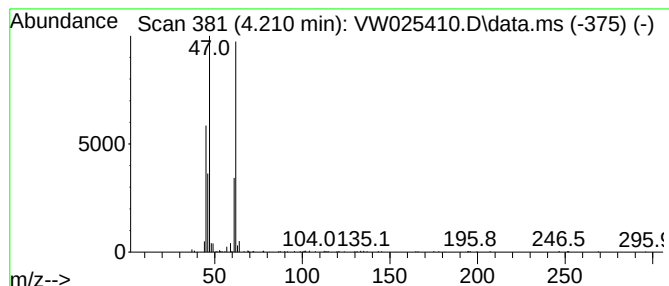
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM030623SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 Dimethyl sulfide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.210	1.77 ug/L	187578	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	94
2			Dimethyl sulfide	62	C2H6S	000075-18-3	91
3			Dimethyl sulfide	62	C2H6S	000075-18-3	91
4			Dimethyl sulfide	62	C2H6S	000075-18-3	91
5			Dimethyl sulfide	62	C2H6S	000075-18-3	91



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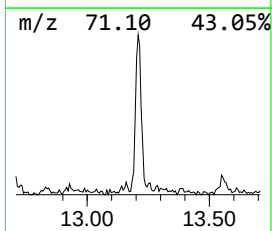
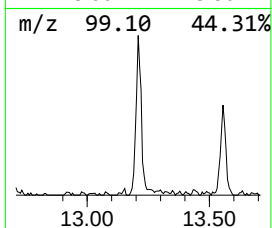
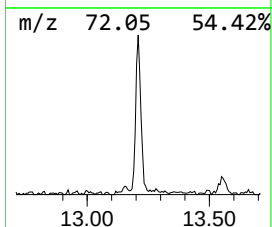
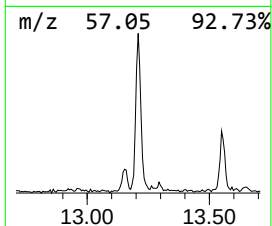
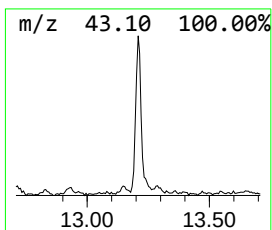
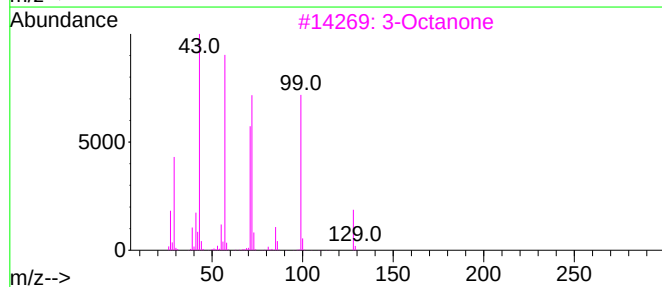
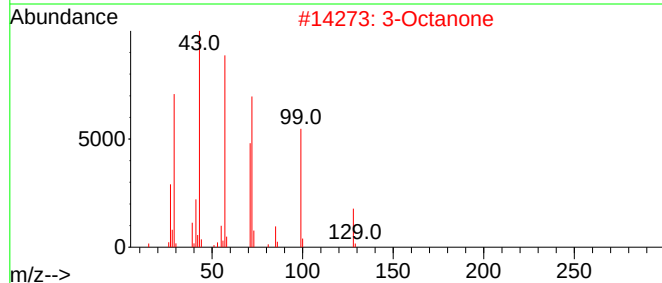
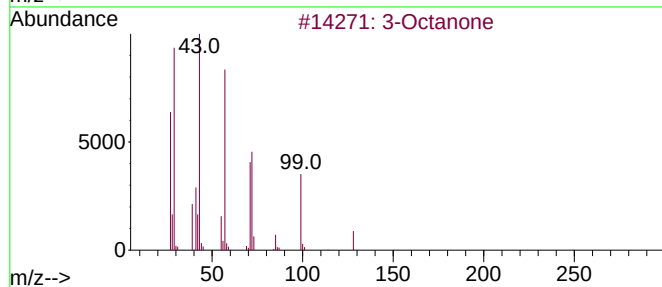
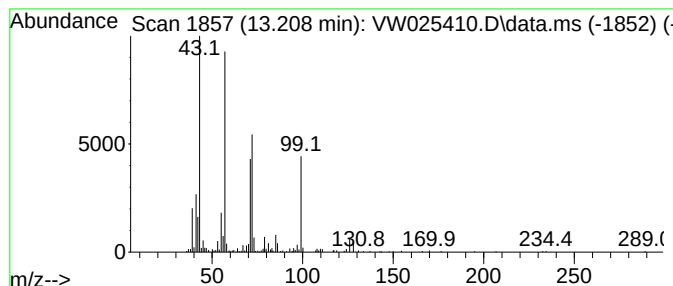
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Quant Title : SFAM01.0

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

Peak Number 3 3-Octanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.208	1.69 ug/L	140888	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanone			128	C8H16O	000106-68-3	78
2	3-Octanone			128	C8H16O	000106-68-3	64
3	3-Octanone			128	C8H16O	000106-68-3	64
4	2,2-Dimethyl-3-octanone			156	C10H20O	005340-64-7	47
5	2,3-Octanedione			142	C8H14O2	000585-25-1	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
Dimethyl sulfide	4.210	1.8	ug/L	187578	1	8.843	2643430	25.0
3-Octanone	13.208	1.7	ug/L	140888	3	13.556	2081390	25.0