

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW102723\
 Data File : VW027470.D
 Acq On : 27 Oct 2023 17:08
 Operator : SY/MD
 Sample : 05112-02RE
 Misc : 6.76g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 E0LJ9RE

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\SFAMWLM101123SMA.M
 Title : SFAM01.0

Signal : TIC: VW027470.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	91	rBV	72893	180063	12.77%	2.280%
2	2.893	160	165	182	rVB	63243	176096	12.49%	2.230%
3	3.594	278	280	281	rBV2	1351	1388	0.10%	0.018%
4	3.887	327	328	329	rVB	1496	548	0.04%	0.007%
5	3.930	333	335	339	rBV5	1243	1350	0.10%	0.017%
6	4.021	339	350	363	rBV	149668	447568	31.74%	5.667%
7	4.186	375	377	378	rVB2	1402	685	0.05%	0.009%
8	4.320	397	399	401	rVB3	1236	702	0.05%	0.009%
9	4.387	403	410	415	rBV3	5253	13972	0.99%	0.177%
10	4.570	439	440	441	rBV	949	658	0.05%	0.008%
11	4.618	445	448	450	rBV3	1605	1626	0.12%	0.021%
12	4.759	468	471	475	rBV5	1171	1919	0.14%	0.024%
13	4.911	488	496	514	rBV2	36633	130432	9.25%	1.651%
14	5.240	547	550	553	rBV3	1074	1617	0.11%	0.020%
15	5.271	553	555	560	rVB6	1170	1344	0.10%	0.017%
16	5.320	560	563	565	rVB4	792	1108	0.08%	0.014%
17	5.356	565	569	571	rBV5	1296	2047	0.15%	0.026%
18	5.655	616	618	621	rVV4	822	929	0.07%	0.012%
19	5.685	621	623	624	rVB2	1082	585	0.04%	0.007%
20	5.856	650	651	653	rBV2	521	219	0.02%	0.003%
21	5.880	653	655	656	rBV2	917	577	0.04%	0.007%
22	5.941	656	665	677	rBV6	12369	39929	2.83%	0.506%
23	6.063	683	685	688	rBV4	1079	826	0.06%	0.010%
24	6.088	688	689	693	rVV4	829	1226	0.09%	0.016%
25	6.155	697	700	701	rBV3	911	1081	0.08%	0.014%
26	6.197	705	707	709	rBV3	669	520	0.04%	0.007%
27	6.228	709	712	715	rBV5	551	773	0.05%	0.010%
28	6.264	715	718	720	rBV4	625	600	0.04%	0.008%
29	6.374	734	736	737	rVB	1175	814	0.06%	0.010%
30	6.399	737	740	741	rVB3	976	928	0.07%	0.012%
31	6.429	741	745	747	rBV4	1264	1653	0.12%	0.021%
32	6.460	747	750	752	rBV4	661	757	0.05%	0.010%
33	6.569	766	768	770	rBV3	1069	700	0.05%	0.009%
34	6.685	785	787	788	rBV2	655	369	0.03%	0.005%
35	6.716	790	792	793	rBV2	1033	563	0.04%	0.007%
36	6.801	803	806	807	rBV3	696	531	0.04%	0.007%

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 Title : SFAM01.0

37	6.862	814	816	818	rBV3	733	620	0.04%	0.008%
38	6.880	818	819	821	rBV	931	569	0.04%	0.007%
39	6.899	821	822	823	rBV	1328	800	0.06%	0.010%
40	6.966	830	833	834	rBV3	1239	1023	0.07%	0.013%
41	7.075	843	851	859	rBV	67200	191750	13.60%	2.428%
42	7.277	883	884	885	rBV	1139	525	0.04%	0.007%
43	7.441	909	911	913	rBV3	1071	742	0.05%	0.009%
44	7.551	926	929	931	rBV3	1404	1288	0.09%	0.016%
45	7.648	935	945	958	rVV	254817	632499	44.85%	8.008%
46	7.862	978	980	982	rVB3	1541	1395	0.10%	0.018%
47	7.880	982	983	985	rBV2	1123	1036	0.07%	0.013%
48	7.965	996	997	998	rVB	1396	511	0.04%	0.006%
49	8.051	1010	1011	1013	rVB2	1094	666	0.05%	0.008%
50	8.276	1038	1048	1065	rBV2	476970	1410238	100.00%	17.855%
51	8.642	1105	1108	1109	rBV3	945	1071	0.08%	0.014%
52	8.782	1127	1131	1132	rBV3	1182	1515	0.11%	0.019%
53	8.843	1133	1141	1152	rVB	443290	889963	63.11%	11.268%
54	9.032	1171	1172	1173	rBV	1120	580	0.04%	0.007%
55	9.276	1203	1212	1221	rBV	337771	701349	49.73%	8.880%
56	9.587	1261	1263	1264	rBV2	774	655	0.05%	0.008%
57	9.599	1264	1265	1267	rVV2	676	509	0.04%	0.006%
58	9.666	1272	1276	1281	rVV8	2719	4502	0.32%	0.057%
59	9.746	1286	1289	1291	rVV4	839	999	0.07%	0.013%
60	9.819	1300	1301	1304	rBV3	1103	1069	0.08%	0.014%
61	9.861	1307	1308	1309	rBV	648	335	0.02%	0.004%
62	10.032	1330	1336	1348	rVB	127945	231679	16.43%	2.933%
63	10.258	1372	1373	1374	rBV	1086	612	0.04%	0.008%
64	10.325	1376	1384	1390	rBV	436852	780406	55.34%	9.881%
65	10.575	1420	1425	1432	rBV	63979	111029	7.87%	1.406%
66	10.855	1466	1471	1475	rBV7	2716	6081	0.43%	0.077%
67	10.922	1475	1482	1497	rVV	216553	375816	26.65%	4.758%
68	11.282	1540	1541	1543	rVB2	1335	629	0.04%	0.008%
69	11.392	1557	1559	1560	rBV2	1347	759	0.05%	0.010%
70	11.501	1575	1577	1578	rBV2	1042	630	0.04%	0.008%
71	11.629	1588	1598	1608	rBV	350661	594559	42.16%	7.528%
72	11.715	1611	1612	1613	rBV	1901	1124	0.08%	0.014%
73	11.831	1627	1631	1637	rBV8	3315	6993	0.50%	0.089%
74	11.989	1655	1657	1659	rBV3	597	623	0.04%	0.008%
75	12.099	1674	1675	1678	rBV3	929	1169	0.08%	0.015%
76	12.172	1684	1687	1688	rBV3	1613	1484	0.11%	0.019%

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 Title : SFAM01.0

77	12.245	1696	1699	1700	rBV3	880	764	0.05%	0.010%
78	12.337	1709	1714	1715	rBV5	1857	2055	0.15%	0.026%
79	12.416	1724	1727	1728	rBV3	1418	1075	0.08%	0.014%
80	12.519	1742	1744	1745	rVB2	778	500	0.04%	0.006%
81	12.532	1745	1746	1747	rBV	1176	694	0.05%	0.009%
82	12.599	1752	1757	1764	rVB2	8910	18662	1.32%	0.236%
83	12.690	1764	1772	1779	rBV	229878	371466	26.34%	4.703%
84	12.867	1800	1801	1802	rBV	1121	772	0.05%	0.010%
85	12.928	1808	1811	1813	rBV4	2157	2395	0.17%	0.030%
86	13.172	1850	1851	1854	rVB3	745	473	0.03%	0.006%
87	13.239	1857	1862	1865	rBV6	1298	2974	0.21%	0.038%
88	13.391	1886	1887	1891	rBV4	1328	1844	0.13%	0.023%
89	13.501	1895	1905	1908	rBV3	9020	18058	1.28%	0.229%
90	13.556	1908	1914	1923	rVV	141942	225421	15.98%	2.854%
91	13.647	1923	1929	1936	rVV2	14350	26136	1.85%	0.331%
92	13.848	1955	1962	1968	rBV	125764	208627	14.79%	2.641%
93	14.324	2036	2040	2041	rBV4	1717	2459	0.17%	0.031%
94	14.519	2068	2072	2081	rVB8	4524	9430	0.67%	0.119%
95	15.019	2152	2154	2155	rBV2	1461	810	0.06%	0.010%
96	15.202	2179	2184	2191	rBV5	4764	10443	0.74%	0.132%
97	15.482	2224	2230	2234	rBV	4874	10248	0.73%	0.130%
98	16.214	2348	2350	2355	rBV6	1859	2851	0.20%	0.036%
99	16.379	2375	2377	2379	rBV3	1226	802	0.06%	0.010%
100	16.421	2381	2384	2387	rBV5	1842	2814	0.20%	0.036%

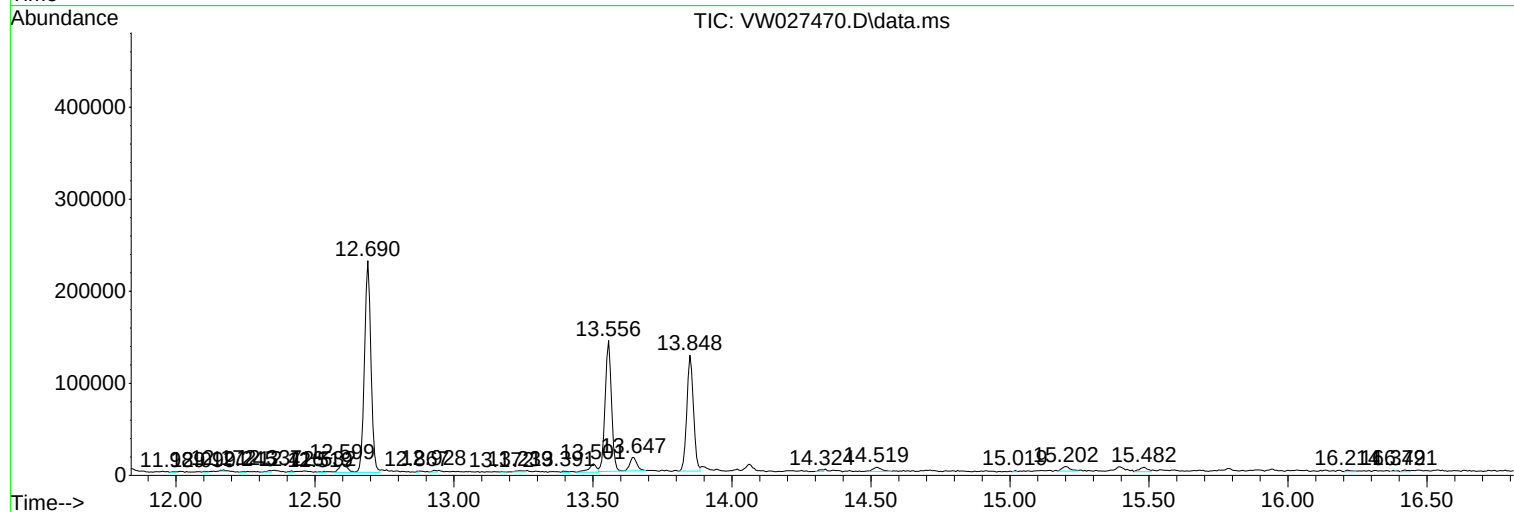
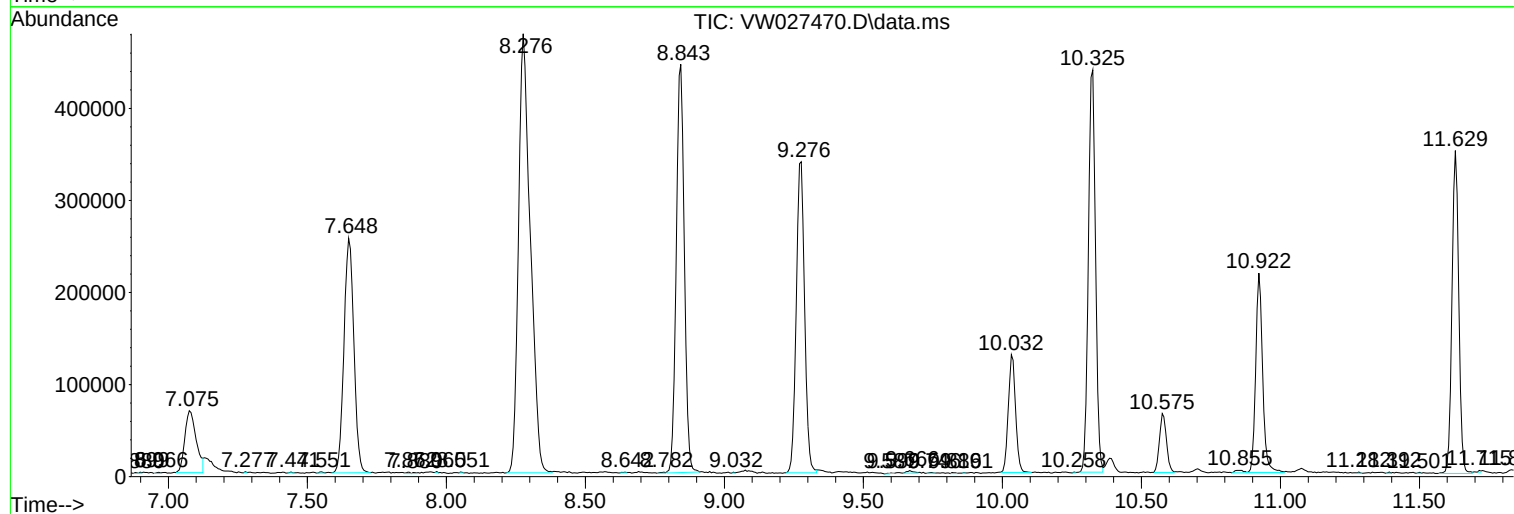
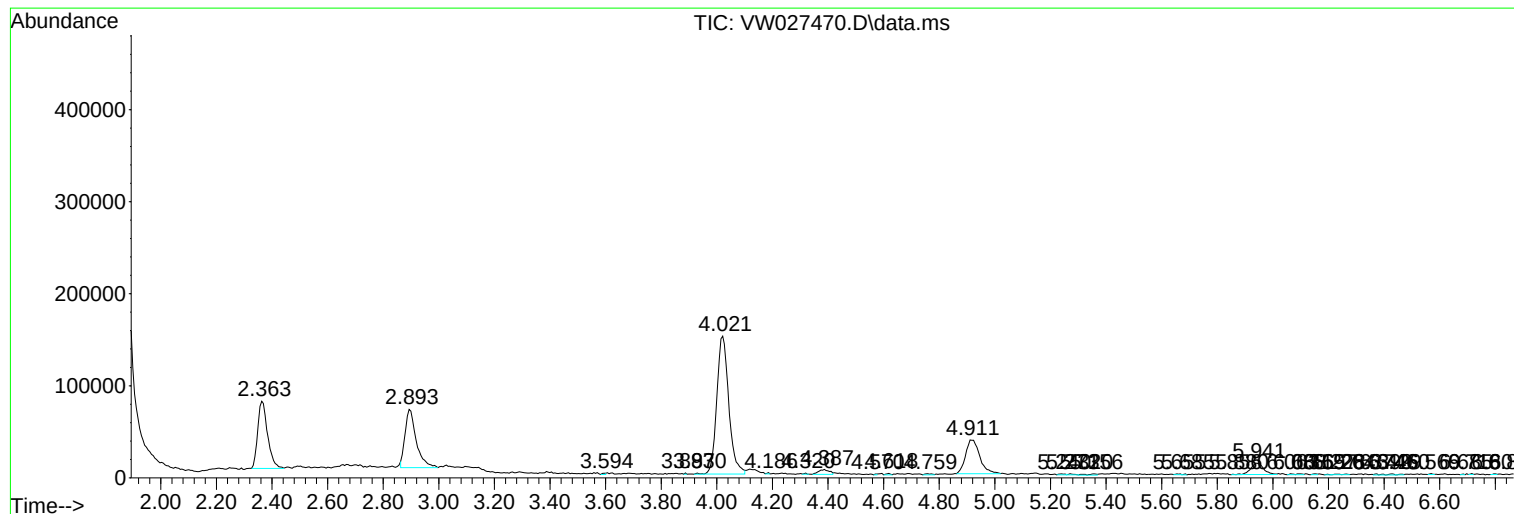
Sum of corrected areas: 7898278

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM101123SMA.M
Quant Title : SFAM01.0

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



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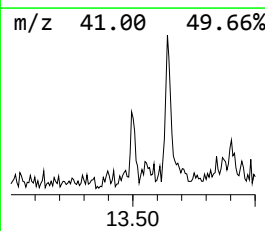
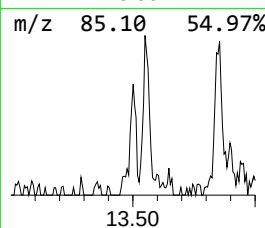
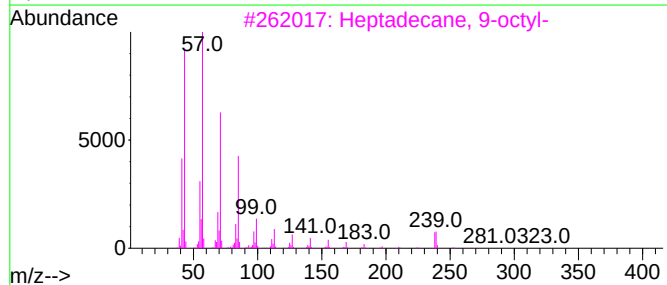
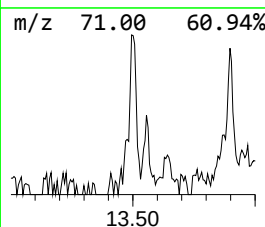
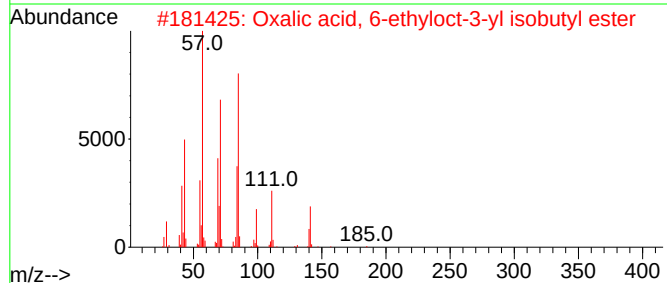
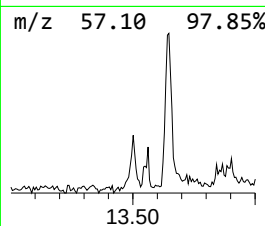
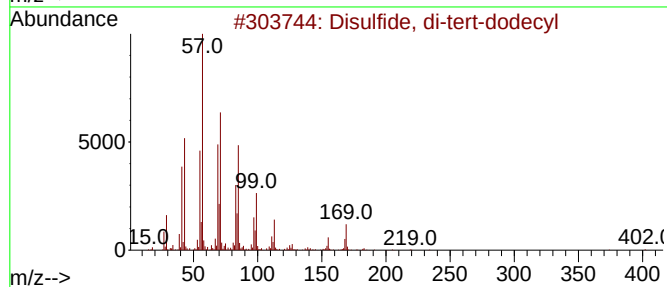
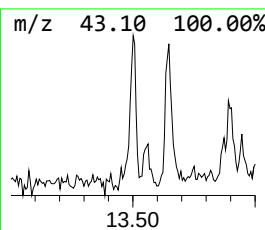
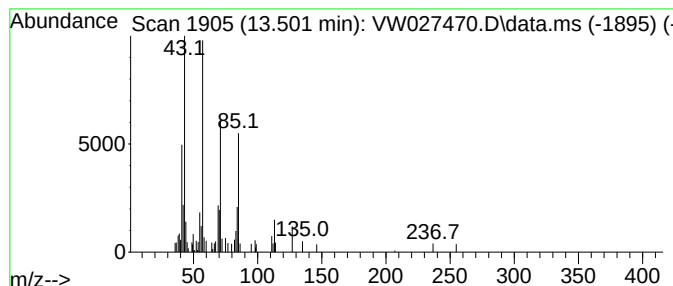
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM101123SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 Disulfide, di-tert-dodecyl Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.501	2.00 ug/L	18058	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disulfide, di-tert-dodecyl	402	C24H50S2	027458-90-8	72
2			Oxalic acid, 6-ethyloct-3-yl iso...	286	C16H30O4	1010309-34-1	64
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	53
4			Pentane, 3-ethyl-2-methyl-	114	C8H18	000609-26-7	52
5			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	52



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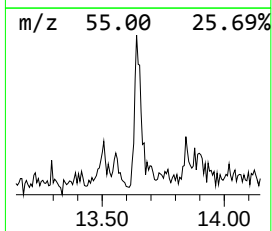
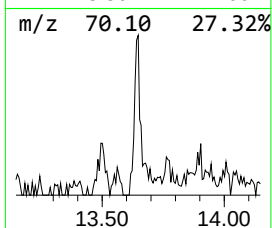
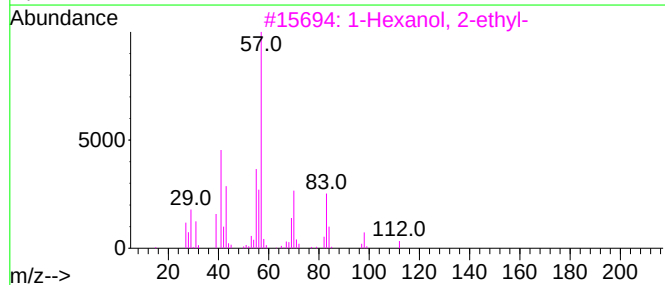
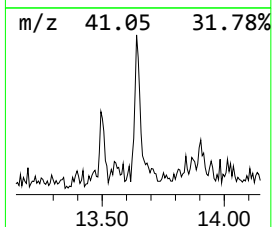
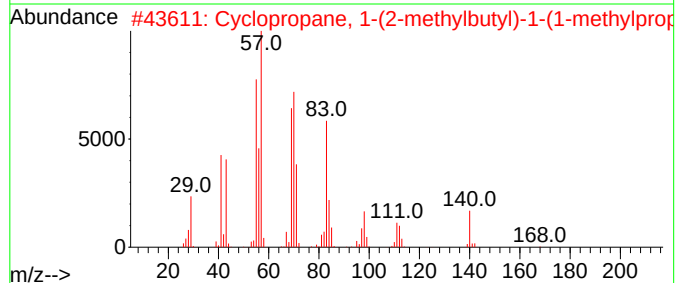
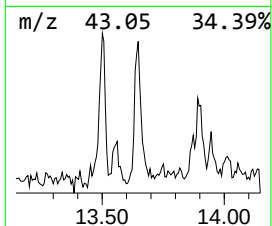
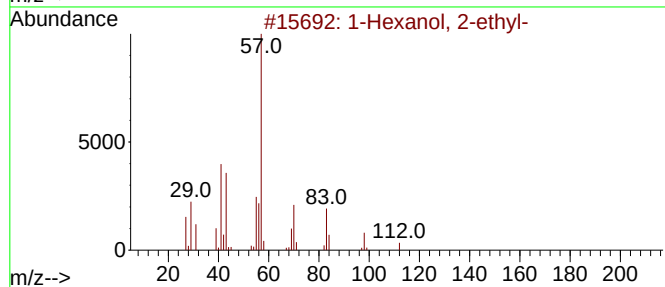
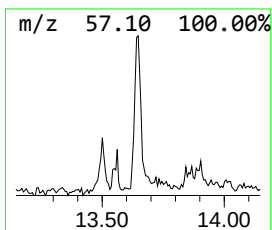
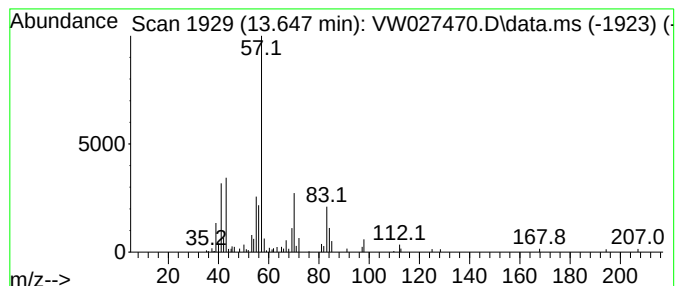
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Quant Title : SFAM01.0

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

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.647	2.90 ug/L	26136	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	72
2	Cyclopropane, 1-(2-methylbutyl)-...			168	C12H24	064723-36-0	64
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
4	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	59
5	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	56



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Quant Title : SFAM01.0

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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Disulfide, di-t...	13.501	2.0	ug/L	18058	3	13.556	225421	25.0
1-Hexanol, 2-et...	13.647	2.9	ug/L	26136	3	13.556	225421	25.0