

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW062624\
 Data File : VW029358.D
 Acq On : 26 Jun 2024 16:12
 Operator : SY/MD
 Sample : P3080-03
 Misc : 7.67g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 GCL40

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\SFAMWLM061824SMA.M
 Title : SFAM01.0

Signal : TIC: VW029358.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	73	78	95	rVB2	49283	137667	10.42%	1.325%
2	2.893	158	165	182	rBV	50745	152074	11.51%	1.463%
3	3.387	241	246	257	rVB4	5623	13827	1.05%	0.133%
4	3.521	265	268	269	rBV3	791	833	0.06%	0.008%
5	4.021	337	350	362	rBV	104992	360192	27.27%	3.466%
6	4.393	403	411	417	rBV3	2999	8772	0.66%	0.084%
7	4.801	476	478	482	rVB2	574	791	0.06%	0.008%
8	4.929	485	499	518	rBV2	29915	136625	10.34%	1.315%
9	5.435	573	582	583	rBV5	2061	3817	0.29%	0.037%
10	5.557	600	602	608	rVB5	719	842	0.06%	0.008%
11	5.722	624	629	630	rBV4	763	859	0.07%	0.008%
12	5.783	630	639	648	rVV5	4187	13441	1.02%	0.129%
13	5.856	650	651	655	rVV4	919	732	0.06%	0.007%
14	5.941	657	665	677	rVV3	8962	28213	2.14%	0.271%
15	6.112	690	693	696	rBV2	551	895	0.07%	0.009%
16	6.240	712	714	716	rVV2	665	796	0.06%	0.008%
17	6.271	716	719	720	rVV3	1081	1171	0.09%	0.011%
18	6.289	720	722	728	rVV5	1183	2101	0.16%	0.020%
19	6.460	748	750	753	rVB4	701	740	0.06%	0.007%
20	6.490	753	755	761	rBV4	647	1135	0.09%	0.011%
21	6.905	815	823	828	rBV8	1771	5922	0.45%	0.057%
22	6.978	833	835	838	rBV4	869	1075	0.08%	0.010%
23	7.075	842	851	865	rBV	58775	177000	13.40%	1.703%
24	7.252	871	880	900	rVB2	162678	417213	31.58%	4.014%
25	7.429	907	909	913	rVB4	680	660	0.05%	0.006%
26	7.648	935	945	959	rBV	235973	574003	43.45%	5.523%
27	7.923	984	990	992	rBV5	2169	4098	0.31%	0.039%
28	8.020	1003	1006	1008	rBV3	1024	1256	0.10%	0.012%
29	8.154	1020	1028	1037	rVV7	2482	6953	0.53%	0.067%
30	8.276	1037	1048	1065	rBV2	424905	1320997	100.00%	12.710%
31	8.508	1080	1086	1088	rBV6	1364	1861	0.14%	0.018%
32	8.557	1089	1094	1101	rVB7	2435	6758	0.51%	0.065%
33	8.703	1110	1118	1128	rVB5	5471	15405	1.17%	0.148%
34	8.843	1132	1141	1154	rBV	416487	816926	61.84%	7.860%
35	9.063	1173	1177	1178	rBV4	853	1193	0.09%	0.011%
36	9.270	1201	1211	1219	rBV	316992	655335	49.61%	6.306%

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 Title : SFAM01.0

37	9.410	1229	1234	1242	rVB4	5097	10931	0.83%	0.105%
38	9.496	1245	1248	1249	rBV3	862	855	0.06%	0.008%
39	9.587	1260	1263	1266	rBV4	960	1819	0.14%	0.018%
40	9.660	1271	1275	1286	rBV7	2651	5211	0.39%	0.050%
41	9.739	1286	1288	1289	rBV2	713	686	0.05%	0.007%
42	9.776	1293	1294	1300	rVB5	751	766	0.06%	0.007%
43	9.892	1308	1313	1317	rBV5	869	1838	0.14%	0.018%
44	9.953	1319	1323	1328	rBV4	1503	1893	0.14%	0.018%
45	10.032	1329	1336	1346	rBV	147352	275371	20.85%	2.650%
46	10.325	1374	1384	1391	rBV	496324	899527	68.09%	8.655%
47	10.386	1391	1394	1400	rVB	10116	17307	1.31%	0.167%
48	10.502	1407	1413	1418	rVB5	4676	8975	0.68%	0.086%
49	10.575	1419	1425	1434	rBV	96418	169287	12.82%	1.629%
50	10.703	1442	1446	1451	rVB2	7669	12949	0.98%	0.125%
51	10.758	1451	1455	1461	rVB7	1670	3177	0.24%	0.031%
52	10.861	1463	1472	1477	rBV	687925	1204467	91.18%	11.589%
53	10.922	1477	1482	1498	rVV	222279	385115	29.15%	3.706%
54	11.068	1500	1506	1515	rVV	32044	55965	4.24%	0.538%
55	11.172	1521	1523	1527	rVB4	1940	2764	0.21%	0.027%
56	11.331	1547	1549	1555	rVB3	1303	1680	0.13%	0.016%
57	11.404	1557	1561	1563	rBV5	1396	2188	0.17%	0.021%
58	11.495	1574	1576	1577	rBV2	1002	661	0.05%	0.006%
59	11.629	1590	1598	1607	rBV	498806	817399	61.88%	7.865%
60	11.733	1610	1615	1623	rVB5	5197	11111	0.84%	0.107%
61	11.837	1626	1632	1637	rBV4	6044	12572	0.95%	0.121%
62	12.032	1659	1664	1668	rBV7	627	1326	0.10%	0.013%
63	12.123	1674	1679	1680	rBV5	1429	2034	0.15%	0.020%
64	12.160	1680	1685	1691	rVV7	2805	5750	0.44%	0.055%
65	12.294	1703	1707	1708	rBV4	590	750	0.06%	0.007%
66	12.337	1708	1714	1725	rBV7	5393	12500	0.95%	0.120%
67	12.465	1731	1735	1742	rVV6	3599	7214	0.55%	0.069%
68	12.599	1752	1757	1762	rVB3	9192	16337	1.24%	0.157%
69	12.690	1765	1772	1780	rVV	261184	427206	32.34%	4.111%
70	12.922	1807	1810	1815	rBV6	3812	7454	0.56%	0.072%
71	13.038	1826	1829	1831	rVB4	1150	1305	0.10%	0.013%
72	13.068	1831	1834	1835	rBV4	1040	1035	0.08%	0.010%
73	13.190	1850	1854	1859	rVB4	2347	3057	0.23%	0.029%
74	13.245	1859	1863	1867	rBV3	3015	4684	0.35%	0.045%
75	13.397	1878	1888	1894	rBV4	7702	16935	1.28%	0.163%
76	13.501	1902	1905	1907	rBV3	2293	2883	0.22%	0.028%

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 Title : SFAM01.0

77	13.556	1907	1914	1925	rVV	325079	524771	39.73%	5.049%
78	13.641	1925	1928	1936	rVB	7008	12831	0.97%	0.123%
79	13.702	1936	1938	1941	rBV4	684	691	0.05%	0.007%
80	13.751	1943	1946	1950	rBV4	2080	2937	0.22%	0.028%
81	13.848	1955	1962	1976	rVV	293605	489517	37.06%	4.710%
82	13.946	1976	1978	1983	rVB5	2064	2306	0.17%	0.022%
83	14.013	1985	1989	1991	rBV5	1298	2190	0.17%	0.021%
84	14.062	1992	1997	2005	rVB2	9672	17747	1.34%	0.171%
85	14.239	2024	2026	2027	rBV3	1132	863	0.07%	0.008%
86	14.324	2034	2040	2044	rBV4	6844	12201	0.92%	0.117%
87	14.379	2046	2049	2050	rBV4	920	993	0.08%	0.010%
88	14.690	2097	2100	2101	rBV2	1165	1148	0.09%	0.011%
89	14.714	2102	2104	2111	rVB5	3629	4658	0.35%	0.045%
90	14.879	2128	2131	2134	rBV3	871	1336	0.10%	0.013%
91	15.086	2163	2165	2169	rBV4	830	1209	0.09%	0.012%
92	15.177	2174	2180	2182	rBV7	2282	4256	0.32%	0.041%
93	15.348	2205	2208	2210	rBV4	757	986	0.07%	0.009%
94	15.476	2224	2229	2237	rBV2	9591	16908	1.28%	0.163%
95	15.787	2276	2280	2285	rVB6	1236	2574	0.19%	0.025%
96	15.946	2300	2306	2307	rBV6	1186	1866	0.14%	0.018%
97	16.074	2325	2327	2331	rBV4	816	1505	0.11%	0.014%
98	16.165	2339	2342	2343	rBV3	830	789	0.06%	0.008%
99	16.232	2349	2353	2356	rVV5	482	796	0.06%	0.008%
100	16.586	2408	2411	2412	rBV3	669	748	0.06%	0.007%

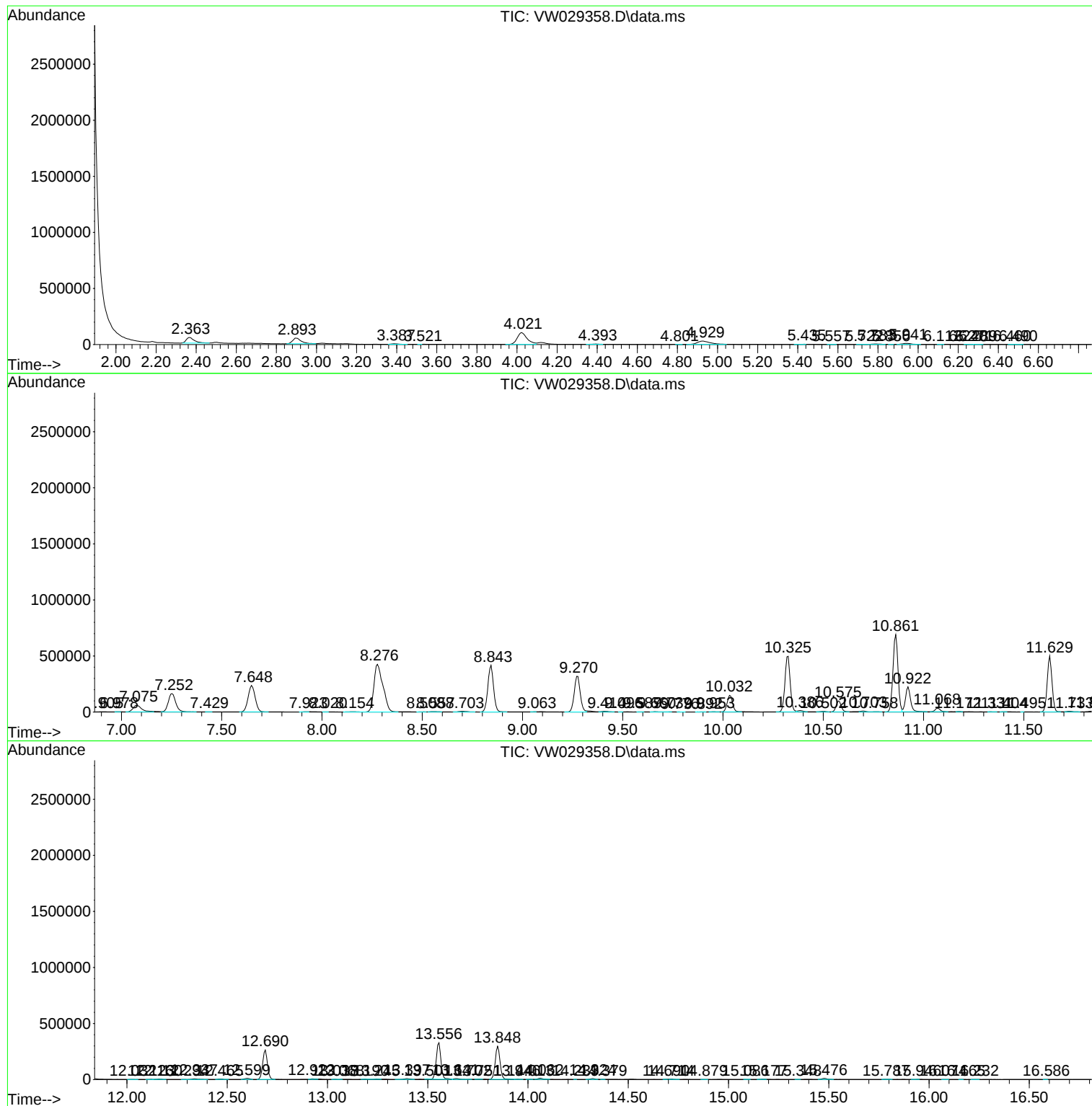
Sum of corrected areas: 10392988

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM061824SMA.M
Quant Title : SFAM01.0

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



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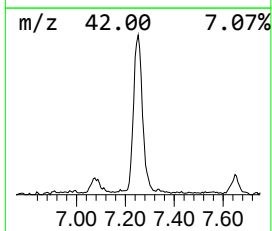
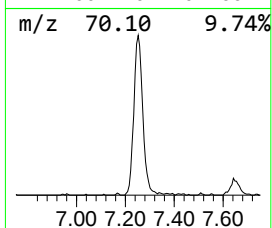
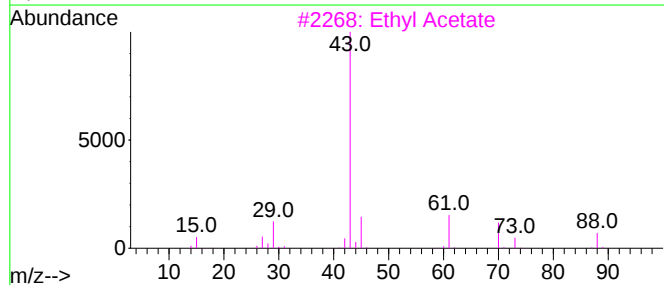
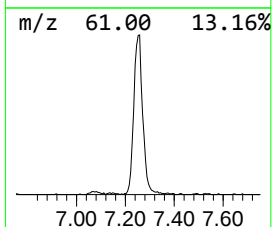
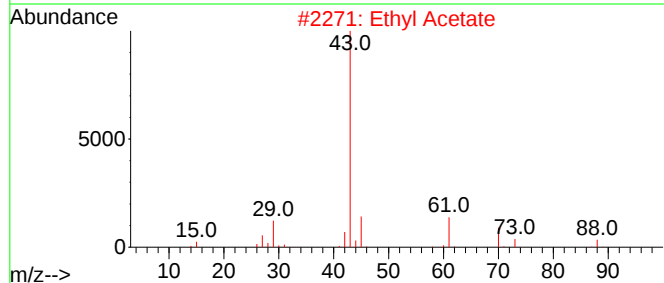
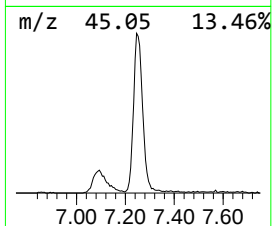
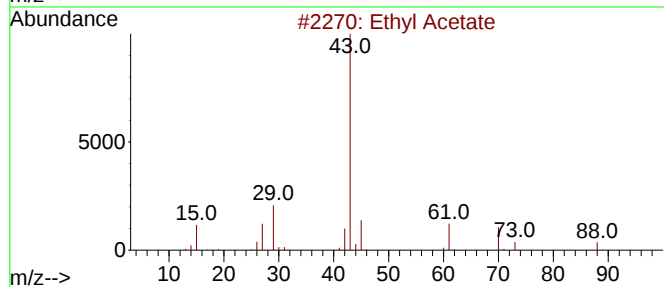
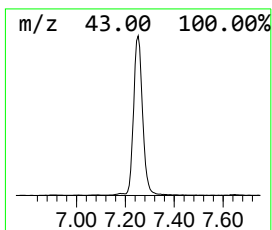
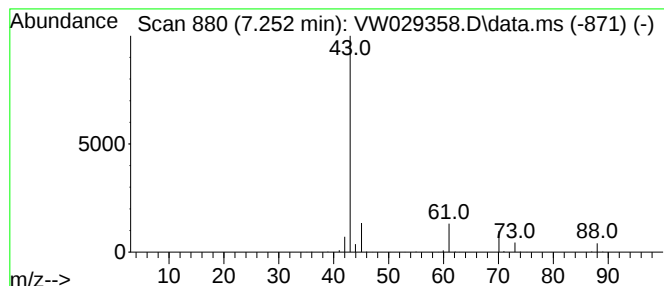
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM061824SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 Ethyl Acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.252	12.77 ug/L	417213	1,4-Difluorobenzene	8.843

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Acetate	88	C4H8O2	000141-78-6	90
2			Ethyl Acetate	88	C4H8O2	000141-78-6	90
3			Ethyl Acetate	88	C4H8O2	000141-78-6	64
4			Ethyl Acetate	88	C4H8O2	000141-78-6	59
5			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	42



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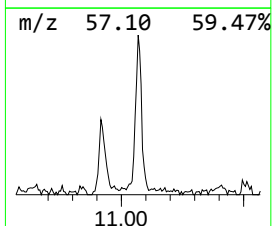
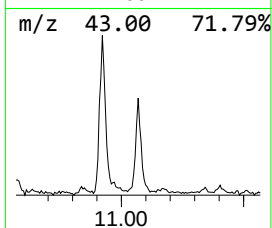
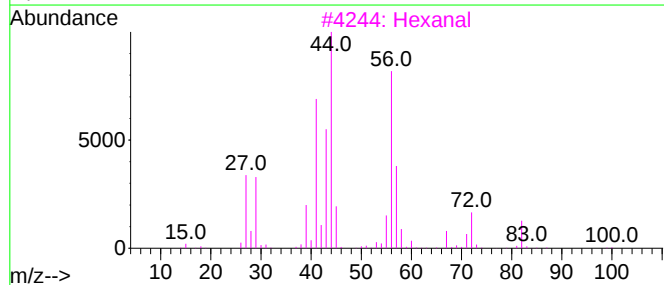
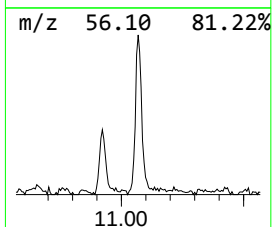
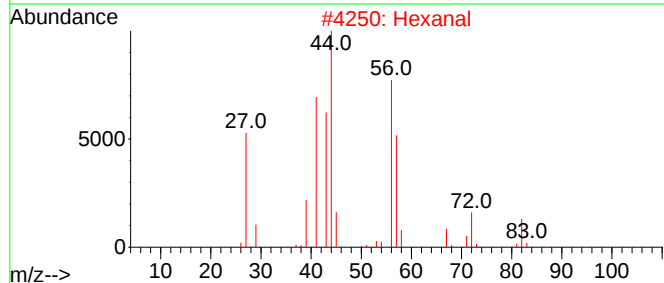
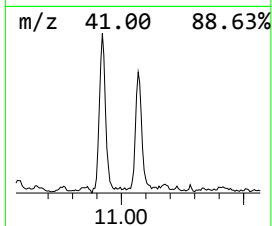
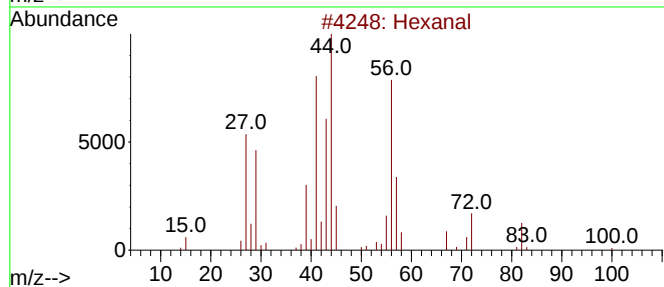
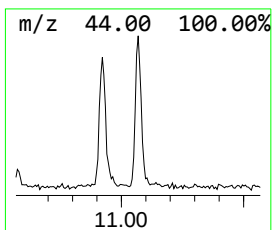
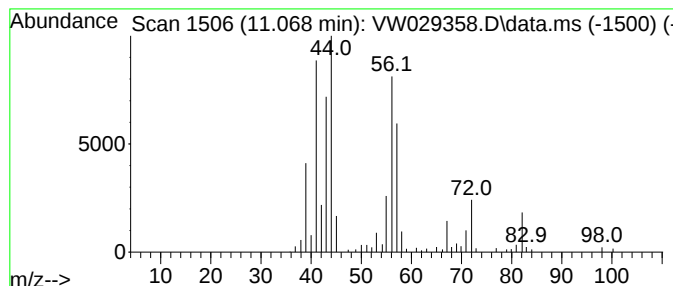
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Quant Title : SFAM01.0

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

Peak Number 3 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.069	1.71 ug/L	55965	Chlorobenzene-d5	11.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	81
2	Hexanal			100	C6H12O	000066-25-1	64
3	Hexanal			100	C6H12O	000066-25-1	59
4	Hexanal			100	C6H12O	000066-25-1	52
5	Hexanal			100	C6H12O	000066-25-1	46



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethyl Acetate	7.252	12.8	ug/L	417213	1	8.843	816926	25.0
Hexanal	11.069	1.7	ug/L	55965	2	11.629	817399	25.0