

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW071522\
 Data File : VW023804.D
 Acq On : 16 Jul 2022 21:37
 Operator : SY/VA
 Sample : N3702-18
 Misc : 6.33g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 F5C72

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\SFAMWLM071322SMA.M
 Title : SFAM01.0

Signal : TIC: VW023804.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.239	47	55	57	rBV6	11059	29271	0.81%	0.279%
2	2.349	68	73	82	rVB2	117830	204779	5.68%	1.955%
3	2.873	156	159	171	rVB	55822	119865	3.33%	1.144%
4	3.501	260	262	263	rBV2	1425	1074	0.03%	0.010%
5	3.641	282	285	289	rVB5	1546	1602	0.04%	0.015%
6	3.867	318	322	323	rBV4	900	1297	0.04%	0.012%
7	4.013	336	346	358	rBV3	43974	140860	3.91%	1.345%
8	4.251	382	385	388	rBV5	1636	2563	0.07%	0.024%
9	4.348	398	401	404	rVB4	1154	1098	0.03%	0.010%
10	4.409	404	411	412	rBV4	3737	6815	0.19%	0.065%
11	4.696	454	458	459	rBV3	1010	1212	0.03%	0.012%
12	5.324	558	561	562	rBV3	1400	1107	0.03%	0.011%
13	5.415	567	576	577	rBV9	4245	8841	0.25%	0.084%
14	5.745	628	630	632	rVV2	1658	1219	0.03%	0.012%
15	5.915	652	658	660	rBV6	2147	3376	0.09%	0.032%
16	6.110	689	690	691	rBV	1497	924	0.03%	0.009%
17	6.190	702	703	706	rBV3	982	1134	0.03%	0.011%
18	6.238	710	711	714	rVB3	1427	1193	0.03%	0.011%
19	6.385	733	735	739	rVB4	1122	1608	0.04%	0.015%
20	6.421	739	741	743	rBV3	941	1212	0.03%	0.012%
21	6.543	758	761	767	rBV7	1296	2615	0.07%	0.025%
22	6.586	767	768	770	rVB2	1742	1134	0.03%	0.011%
23	6.671	779	782	784	rVB4	1220	1376	0.04%	0.013%
24	6.708	784	788	790	rBV5	1087	1431	0.04%	0.014%
25	6.927	822	824	826	rBV2	986	1156	0.03%	0.011%
26	7.080	842	849	854	rBV	23212	56175	1.56%	0.536%
27	7.165	856	863	879	rVB	253642	658129	18.27%	6.282%
28	7.397	899	901	904	rBV4	1038	1058	0.03%	0.010%
29	7.549	923	926	930	rBV6	1403	1731	0.05%	0.017%
30	7.647	934	942	953	rVB	116846	284567	7.90%	2.716%
31	7.939	985	990	998	rVB8	3845	10547	0.29%	0.101%
32	8.275	1032	1045	1059	rBV2	211730	672449	18.66%	6.419%
33	8.610	1098	1100	1101	rBV2	1319	1191	0.03%	0.011%
34	8.787	1127	1129	1130	rBV2	1279	1231	0.03%	0.012%
35	8.842	1130	1138	1152	rVV	259341	496791	13.79%	4.742%
36	9.092	1170	1179	1188	rVV	407517	800519	22.22%	7.642%

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Integrator: RTE

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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\SFAMWLM071322SMA.M
 Title : SFAM01.0

37	9.274	1201	1209	1219	rVB	166685	330830	9.18%	3.158%
38	9.341	1219	1220	1225	rVB5	1574	1391	0.04%	0.013%
39	9.646	1268	1270	1271	rBV2	1293	1053	0.03%	0.010%
40	9.756	1287	1288	1290	rBV2	1602	1076	0.03%	0.010%
41	9.811	1293	1297	1299	rBV5	1173	1353	0.04%	0.013%
42	9.835	1299	1301	1303	rBV3	1395	1300	0.04%	0.012%
43	9.988	1324	1326	1327	rVV2	2082	1537	0.04%	0.015%
44	10.036	1327	1334	1344	rVB	72708	135942	3.77%	1.298%
45	10.122	1346	1348	1352	rVB5	1814	2300	0.06%	0.022%
46	10.207	1358	1362	1365	rBV6	2552	4158	0.12%	0.040%
47	10.323	1373	1381	1389	rBV	298136	517577	14.37%	4.941%
48	10.579	1416	1423	1433	rVB	51690	90803	2.52%	0.867%
49	10.707	1437	1444	1450	rBV2	6682	13785	0.38%	0.132%
50	10.860	1460	1469	1475	rBV	2170616	3602766	100.00%	34.392%
51	10.920	1475	1479	1489	rVB	99049	182940	5.08%	1.746%
52	11.061	1499	1502	1509	rVB2	11959	19948	0.55%	0.190%
53	11.134	1512	1514	1515	rBV2	1350	1150	0.03%	0.011%
54	11.219	1525	1528	1531	rBV5	1104	1772	0.05%	0.017%
55	11.329	1543	1546	1547	rBV2	1296	1405	0.04%	0.013%
56	11.433	1560	1563	1568	rVB6	3445	5263	0.15%	0.050%
57	11.475	1568	1570	1572	rVB3	1272	1028	0.03%	0.010%
58	11.518	1575	1577	1579	rVB3	1802	1049	0.03%	0.010%
59	11.561	1579	1584	1585	rBV5	1303	1989	0.06%	0.019%
60	11.628	1588	1595	1603	rBV	386957	639772	17.76%	6.107%
61	11.945	1645	1647	1650	rBV3	1190	1119	0.03%	0.011%
62	12.036	1659	1662	1664	rBV4	1177	1494	0.04%	0.014%
63	12.140	1677	1679	1681	rBV3	1754	1147	0.03%	0.011%
64	12.164	1681	1683	1685	rBV3	1423	1149	0.03%	0.011%
65	12.329	1705	1710	1712	rBV6	1061	1641	0.05%	0.016%
66	12.603	1749	1755	1760	rVV4	11362	20441	0.57%	0.195%
67	12.688	1763	1769	1777	rVV	159707	263072	7.30%	2.511%
68	12.762	1779	1781	1785	rVB4	1583	1344	0.04%	0.013%
69	12.847	1790	1795	1797	rVB4	993	1424	0.04%	0.014%
70	12.877	1797	1800	1802	rBV4	1873	2171	0.06%	0.021%
71	12.926	1805	1808	1818	rVB10	4350	11473	0.32%	0.110%
72	13.188	1848	1851	1855	rVB3	6346	8598	0.24%	0.082%
73	13.292	1866	1868	1878	rVB6	4930	8926	0.25%	0.085%
74	13.402	1878	1886	1893	rBV4	11242	25913	0.72%	0.247%
75	13.554	1905	1911	1917	rBV	326541	514154	14.27%	4.908%
76	13.761	1939	1945	1953	rBV7	7722	18971	0.53%	0.181%

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Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
 Title : SFAM01.0

77	13.853	1953	1960	1967	rBV	268344	438035	12.16%	4.181%
78	14.066	1991	1995	2007	rVB5	8027	22335	0.62%	0.213%
79	14.200	2014	2017	2020	rBV5	1584	2370	0.07%	0.023%
80	14.310	2032	2035	2036	rBV3	1946	2247	0.06%	0.021%
81	14.493	2060	2065	2068	rBV6	2544	4292	0.12%	0.041%
82	14.633	2084	2088	2090	rBV5	1770	2422	0.07%	0.023%
83	14.719	2098	2102	2105	rVB3	4774	6580	0.18%	0.063%
84	14.786	2111	2113	2117	rVB5	1074	1127	0.03%	0.011%
85	14.828	2117	2120	2124	rBV6	1794	2075	0.06%	0.020%
86	15.023	2150	2152	2154	rBV3	1520	976	0.03%	0.009%
87	15.097	2161	2164	2165	rBV3	1438	1615	0.04%	0.015%
88	15.225	2182	2185	2187	rBV4	2138	2618	0.07%	0.025%
89	15.389	2209	2212	2213	rBV3	1891	1981	0.05%	0.019%
90	15.426	2216	2218	2223	rVB4	3623	5078	0.14%	0.048%
91	15.682	2258	2260	2264	rVB5	1454	1411	0.04%	0.013%
92	15.913	2294	2298	2302	rBV7	792	1649	0.05%	0.016%
93	15.968	2305	2307	2310	rVB3	1649	1461	0.04%	0.014%
94	16.023	2312	2316	2318	rBV4	1082	1852	0.05%	0.018%
95	16.060	2321	2322	2327	rBV5	788	1216	0.03%	0.012%
96	16.249	2350	2353	2357	rBV5	1213	1480	0.04%	0.014%
97	16.432	2381	2383	2385	rVB3	918	908	0.03%	0.009%
98	16.450	2385	2386	2390	rBV4	647	1051	0.03%	0.010%
99	16.712	2426	2429	2430	rVB4	1228	994	0.03%	0.009%
100	16.755	2433	2436	2438	rBV4	1340	1505	0.04%	0.014%

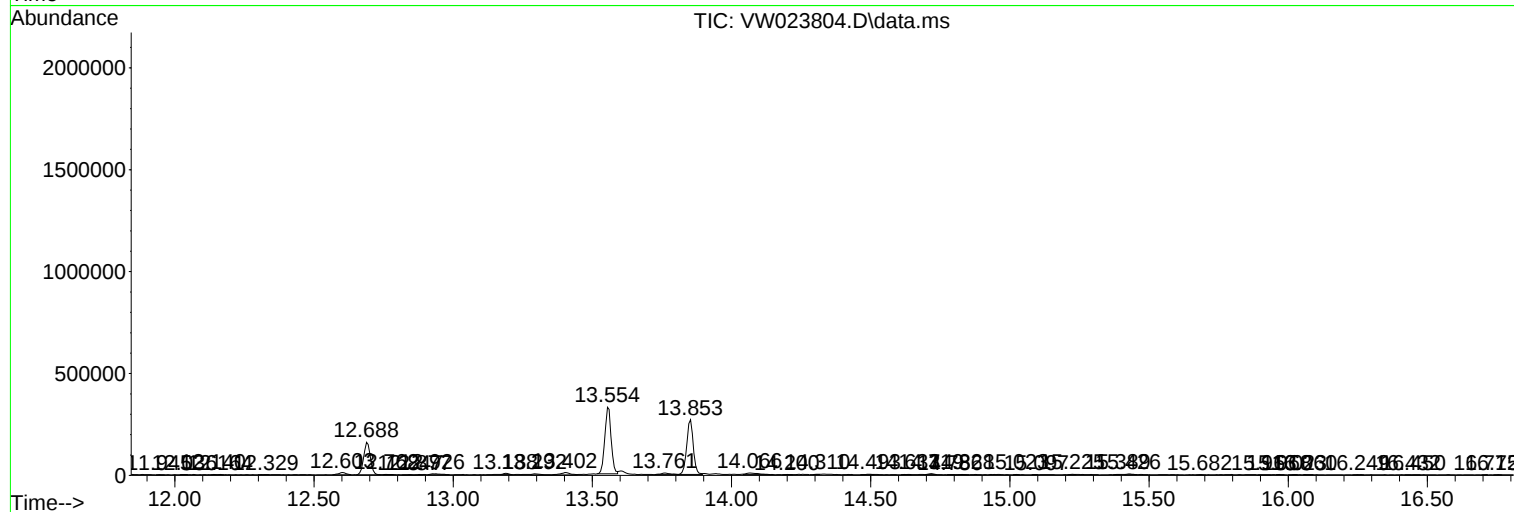
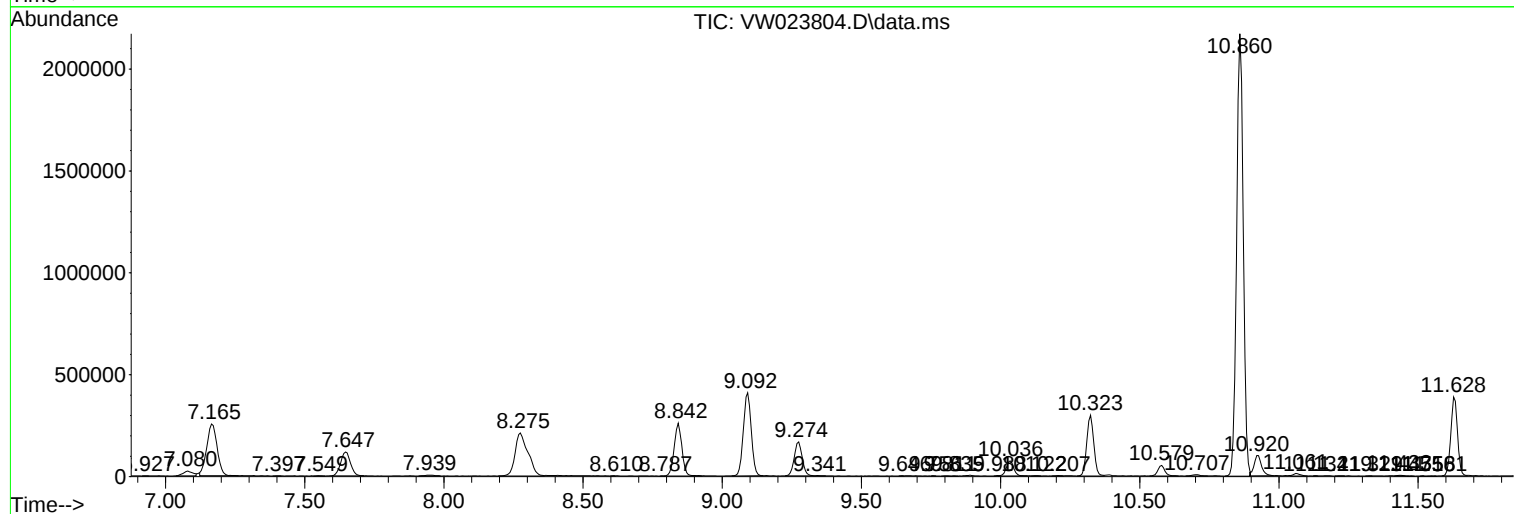
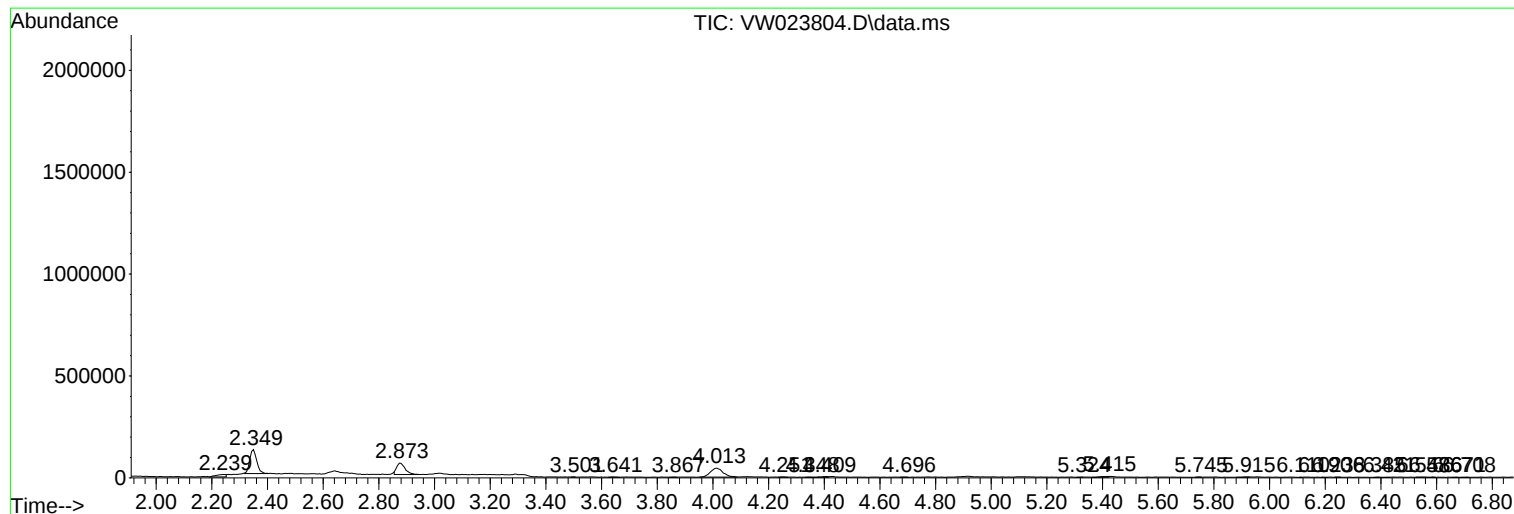
Sum of corrected areas: 10475652

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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



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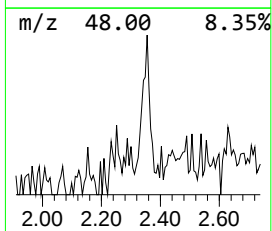
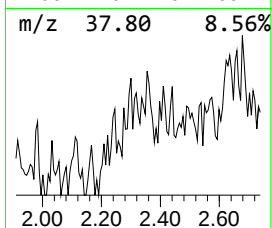
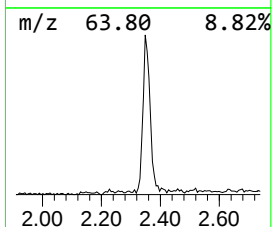
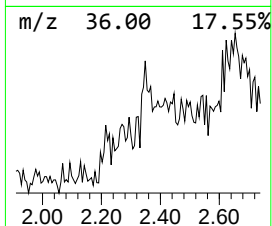
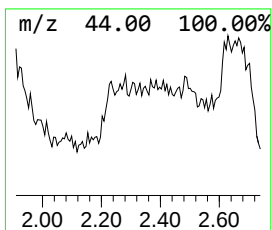
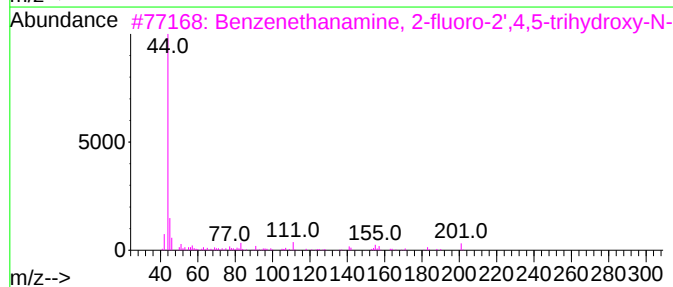
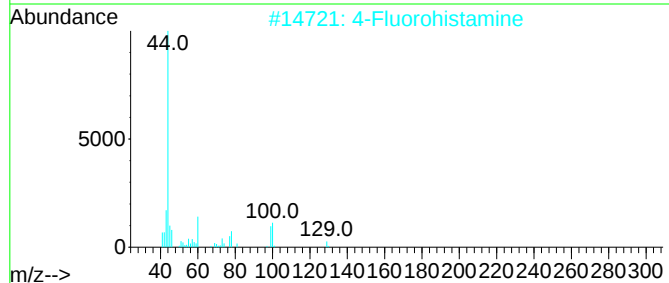
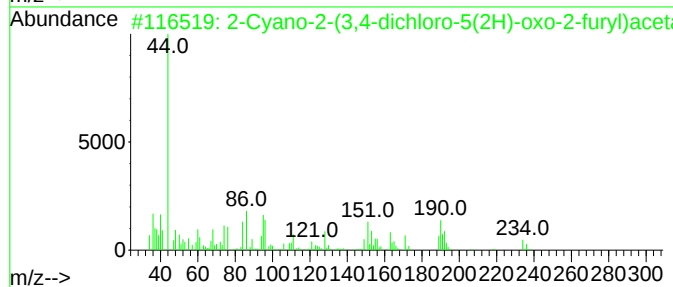
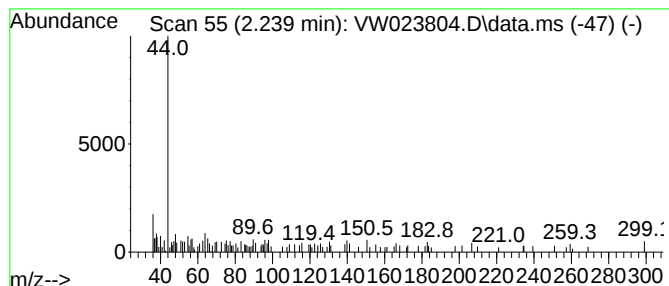
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM071322SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 2-Cyano-2-(3,4-dichloro-5(2... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.239	1.47 ug/L	29271	1,4-Difluorobenzene	8.842

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Cyano-2-(3,4-dichloro-5(2H)-ox...	234	C7H4Cl2N2O3	070097-69-7	56	
2	4-Fluorohistamine	129	C5H8FN3	049872-60-8	53	
3	Benzenethanamine, 2-fluoro-2',4,...	201	C9H12FN03	115562-28-2	53	
4	Hydrastininic acid	251	C11H9N06	000490-25-5	50	
5	1-Pentanol, 4-amino-	103	C5H13NO	000927-55-9	42	



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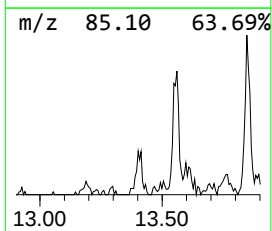
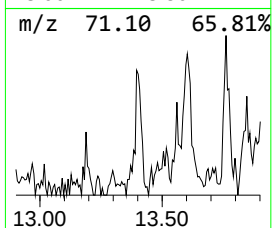
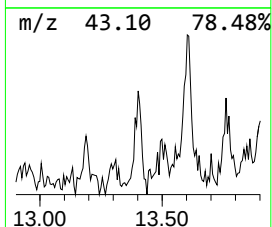
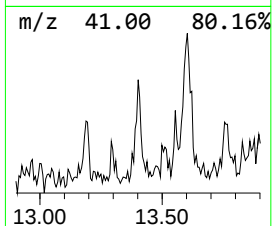
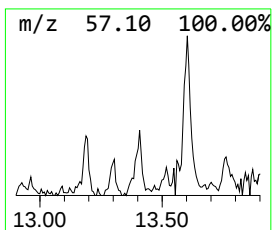
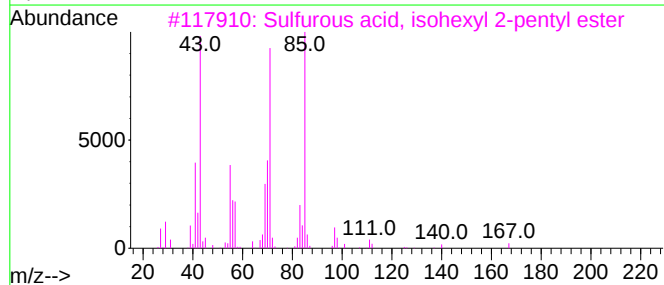
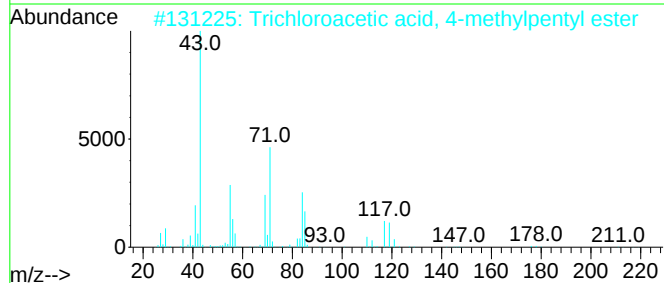
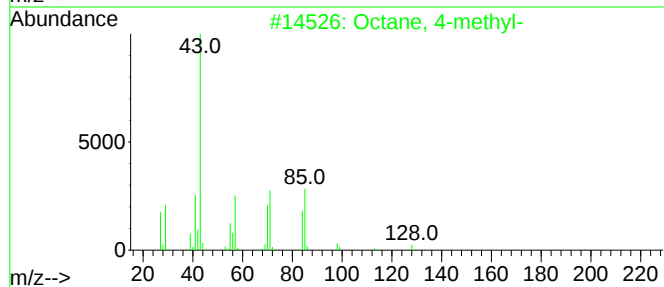
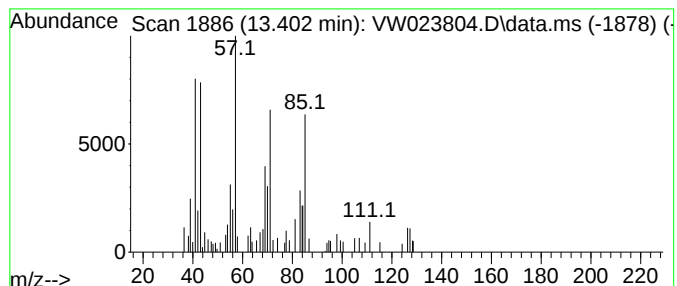
Instrument :
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Quant Title : SFAM01.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.402	1.26 ug/L	25913	1,4-Dichlorobenzene-d4		13.560	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octane, 4-methyl-		128	C9H20	002216-34-4	52
2	Trichloroacetic acid, 4-methylpe...		246	C8H13Cl3O2	1000282-35-2	38
3	Sulfurous acid, isohexyl 2-penty...		236	C11H24O3S	1000309-15-5	38
4	Undecane, 4,7-dimethyl-		184	C13H28	017301-32-5	38
5	Decane, 2,4-dimethyl-		170	C12H26	002801-84-5	35



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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
2-Cyano-2-(3,4-...	2.239	1.5	ug/L	29271	1	8.842	496791	25.0
(DEL) Alkane: S...	13.402	1.3	ug/L	25913	3	13.560	514154	25.0