

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW051022\
 Data File : VW022960.D
 Acq On : 10 May 2022 17:01
 Operator : SY/VA
 Sample : N2766-05
 Misc : 7.21g/10mL/MSVOA_W/SOIL
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 EW4F5

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\SFAMWLM050222SMA.M
 Title : SFAM01.0

Signal : TIC: VW022960.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.965	6	10	15	rVB3	16545	26310	2.83%	0.514%
2	2.184	42	46	49	rVB	9527	13033	1.40%	0.255%
3	2.355	68	74	85	rBV2	141685	243841	26.27%	4.766%
4	2.885	156	161	170	rVB	75718	163692	17.63%	3.199%
5	3.343	234	236	237	rBV2	1281	1106	0.12%	0.022%
6	3.385	238	243	250	rVV3	8742	18702	2.01%	0.366%
7	3.434	250	251	252	rVV	1110	600	0.06%	0.012%
8	3.471	256	257	260	rVV3	1001	586	0.06%	0.011%
9	3.806	310	312	313	rBV2	824	779	0.08%	0.015%
10	3.940	331	334	336	rBV4	1129	1303	0.14%	0.025%
11	4.019	336	347	361	rVV	104076	319469	34.41%	6.244%
12	4.318	395	396	398	rVB2	1344	684	0.07%	0.013%
13	4.379	402	406	407	rBV	2738	3687	0.40%	0.072%
14	4.544	429	433	435	rVB4	1030	1064	0.11%	0.021%
15	4.586	438	440	442	rVB3	804	720	0.08%	0.014%
16	4.763	462	469	471	rBV7	1011	2107	0.23%	0.041%
17	4.916	485	494	495	rBV2	12799	26220	2.82%	0.512%
18	5.098	522	524	527	rBV3	1087	1147	0.12%	0.022%
19	5.129	527	529	530	rBV	960	604	0.07%	0.012%
20	5.287	553	555	557	rBV2	716	779	0.08%	0.015%
21	5.336	561	563	565	rVB3	947	767	0.08%	0.015%
22	5.409	572	575	576	rBV3	1329	1639	0.18%	0.032%
23	5.550	594	598	601	rBV5	1190	1825	0.20%	0.036%
24	5.611	606	608	613	rVB4	992	1169	0.13%	0.023%
25	5.659	613	616	618	rBV4	1225	1580	0.17%	0.031%
26	5.940	654	662	672	rBV9	5872	16066	1.73%	0.314%
27	6.153	694	697	699	rBV3	1024	958	0.10%	0.019%
28	6.415	737	740	742	rBV3	885	1123	0.12%	0.022%
29	6.482	748	751	753	rVB3	1026	982	0.11%	0.019%
30	6.513	753	756	757	rBV2	1405	1060	0.11%	0.021%
31	6.574	764	766	767	rVB	1078	633	0.07%	0.012%
32	6.598	767	770	774	rBV4	1219	2172	0.23%	0.042%
33	6.629	774	775	777	rVV	880	778	0.08%	0.015%
34	6.665	780	781	786	rVV5	781	1175	0.13%	0.023%
35	6.726	789	791	793	rVV2	1071	810	0.09%	0.016%
36	6.873	813	815	816	rBV2	1431	1074	0.12%	0.021%

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 Title : SFAM01.0

37	7.080	840	849	857	rBV	39788	111952	12.06%	2.188%
38	7.519	918	921	922	rBV3	1028	975	0.11%	0.019%
39	7.647	932	942	953	rBV	180111	443340	47.76%	8.665%
40	7.830	969	972	973	rBV3	693	926	0.10%	0.018%
41	8.080	1012	1013	1016	rBV	835	737	0.08%	0.014%
42	8.147	1022	1024	1026	rBV2	1106	1154	0.12%	0.023%
43	8.275	1033	1045	1060	rBV2	300929	928354	100.00%	18.144%
44	8.701	1109	1115	1118	rBV8	1918	3999	0.43%	0.078%
45	8.842	1130	1138	1153	rVB	257286	520427	56.06%	10.171%
46	9.000	1162	1164	1165	rBV2	778	652	0.07%	0.013%
47	9.061	1172	1174	1175	rBV2	1812	1460	0.16%	0.029%
48	9.183	1192	1194	1195	rBV2	1007	761	0.08%	0.015%
49	9.275	1200	1209	1218	rBV	214317	438846	47.27%	8.577%
50	9.512	1246	1248	1250	rBV3	1018	760	0.08%	0.015%
51	9.640	1267	1269	1271	rBV3	874	766	0.08%	0.015%
52	9.835	1300	1301	1303	rBV	851	703	0.08%	0.014%
53	9.884	1306	1309	1314	rVB5	2313	4432	0.48%	0.087%
54	9.927	1314	1316	1317	rBV2	1047	654	0.07%	0.013%
55	10.037	1326	1334	1340	rBV	75681	139462	15.02%	2.726%
56	10.195	1358	1360	1362	rVB3	892	777	0.08%	0.015%
57	10.323	1374	1381	1387	rBV	271674	473793	51.04%	9.260%
58	10.384	1387	1391	1398	rVB	24307	43707	4.71%	0.854%
59	10.579	1417	1423	1430	rVV	36894	65500	7.06%	1.280%
60	10.665	1434	1437	1438	rBV3	1419	1496	0.16%	0.029%
61	10.695	1439	1442	1448	rVB5	3936	7267	0.78%	0.142%
62	10.847	1465	1467	1470	rBV3	1249	1428	0.15%	0.028%
63	10.927	1472	1480	1494	rVV	113636	206832	22.28%	4.042%
64	11.213	1526	1527	1529	rBV2	1297	1173	0.13%	0.023%
65	11.292	1538	1540	1542	rVB2	1121	654	0.07%	0.013%
66	11.335	1542	1547	1548	rBV4	1384	1882	0.20%	0.037%
67	11.408	1558	1559	1561	rBV2	868	677	0.07%	0.013%
68	11.518	1575	1577	1579	rBV3	1015	1021	0.11%	0.020%
69	11.567	1582	1585	1588	rBV2	1164	1765	0.19%	0.034%
70	11.628	1588	1595	1604	rBV	182958	316117	34.05%	6.178%
71	11.786	1619	1621	1624	rBV4	1270	1287	0.14%	0.025%
72	11.835	1625	1629	1635	rVV5	5572	9994	1.08%	0.195%
73	11.908	1639	1641	1647	rVB5	1308	1632	0.18%	0.032%
74	12.164	1679	1683	1689	rBV5	3415	6237	0.67%	0.122%
75	12.341	1709	1712	1713	rBV3	1907	1703	0.18%	0.033%
76	12.609	1751	1756	1761	rVV5	4884	8755	0.94%	0.171%

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 Title : SFAM01.0

77	12.689	1763	1769	1777	rVV	153791	257853	27.78%	5.039%
78	12.762	1780	1781	1785	rVB4	1444	1332	0.14%	0.026%
79	13.036	1825	1826	1834	rBV8	1329	1942	0.21%	0.038%
80	13.195	1849	1852	1853	rVB3	1171	1041	0.11%	0.020%
81	13.231	1855	1858	1859	rBV2	1397	1308	0.14%	0.026%
82	13.554	1905	1911	1920	rBV	62438	100444	10.82%	1.963%
83	13.640	1923	1925	1926	rBV	1961	1789	0.19%	0.035%
84	13.853	1954	1960	1967	rBV2	62836	109473	11.79%	2.140%
85	14.213	2018	2019	2026	rVB6	1413	2250	0.24%	0.044%
86	14.280	2026	2030	2032	rBV4	1006	1668	0.18%	0.033%
87	14.322	2032	2037	2042	rBV7	2625	4956	0.53%	0.097%
88	14.475	2060	2062	2065	rBV4	1145	999	0.11%	0.020%
89	14.597	2080	2082	2084	rBV3	803	667	0.07%	0.013%
90	14.853	2121	2124	2127	rBV5	1178	1531	0.16%	0.030%
91	14.926	2134	2136	2137	rBV2	1329	891	0.10%	0.017%
92	15.030	2151	2153	2155	rBV3	1087	1243	0.13%	0.024%
93	15.310	2194	2199	2200	rBV4	1141	1992	0.21%	0.039%
94	15.359	2204	2207	2212	rVB4	3325	5537	0.60%	0.108%
95	15.761	2271	2273	2274	rBV2	1510	1011	0.11%	0.020%
96	16.036	2317	2318	2320	rBV2	898	614	0.07%	0.012%
97	16.328	2363	2366	2367	rBV2	1021	896	0.10%	0.018%
98	16.548	2400	2402	2404	rBV3	1227	1345	0.14%	0.026%
99	16.609	2409	2412	2413	rBV3	1060	980	0.11%	0.019%
100	16.761	2436	2437	2439	rVV2	1179	624	0.07%	0.012%

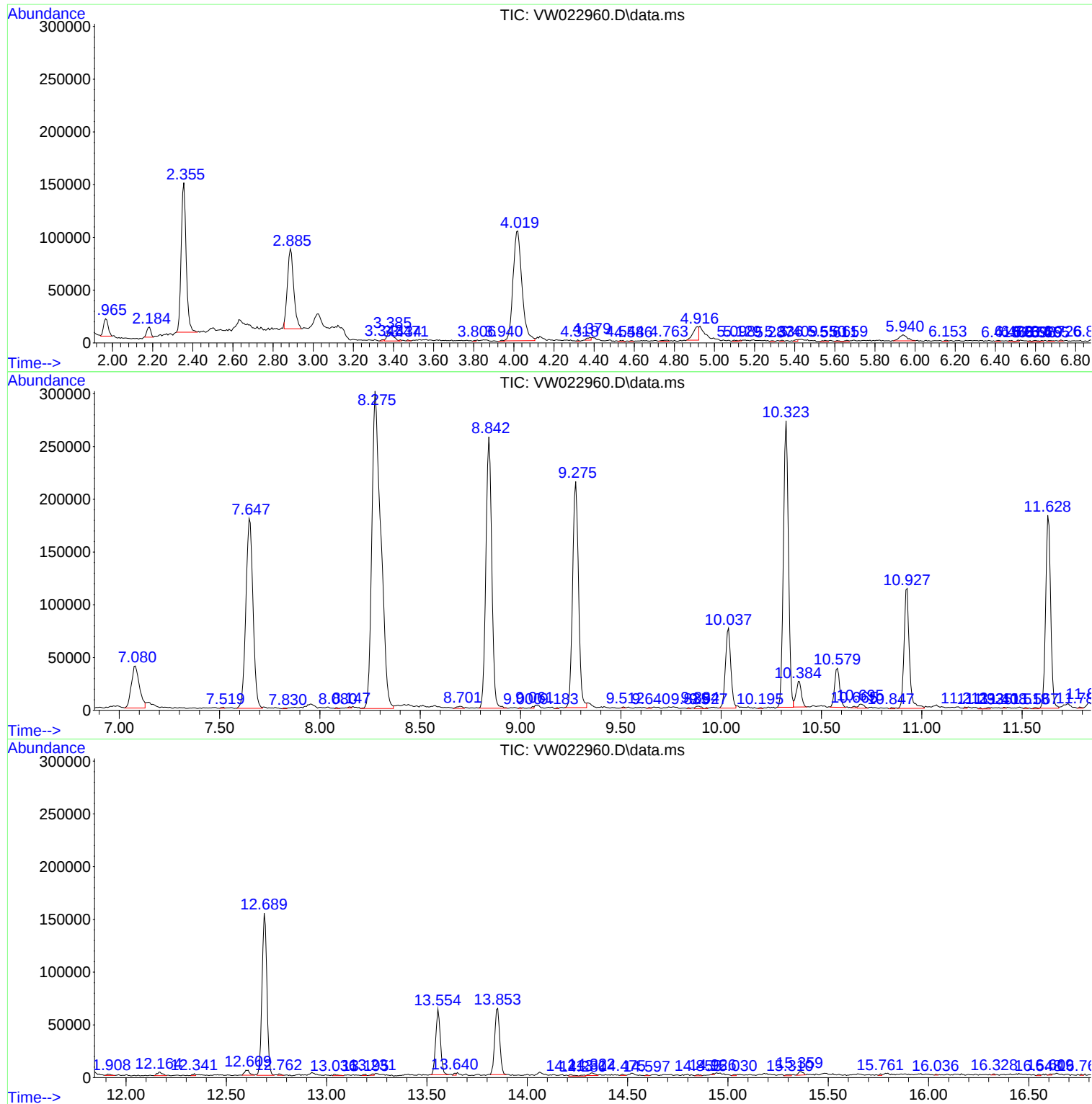
Sum of corrected areas: 5116687

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050222SMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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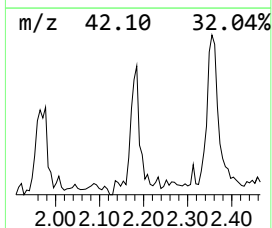
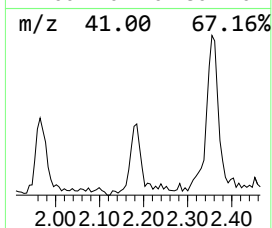
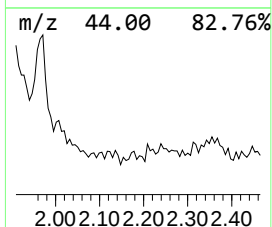
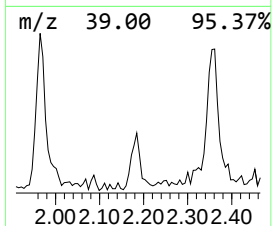
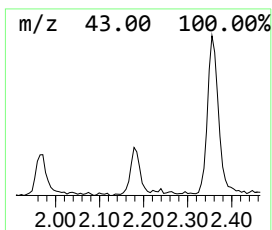
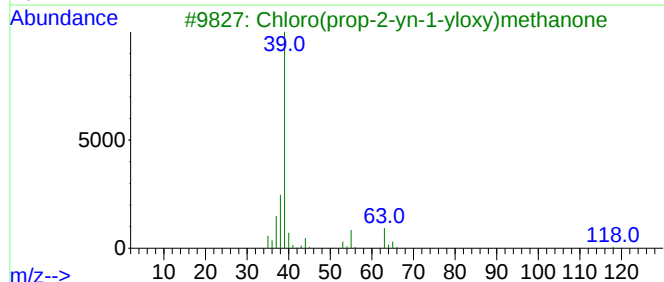
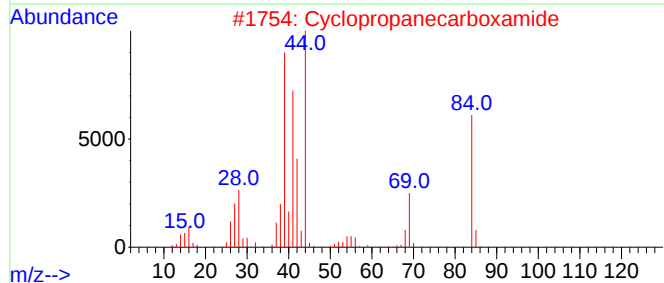
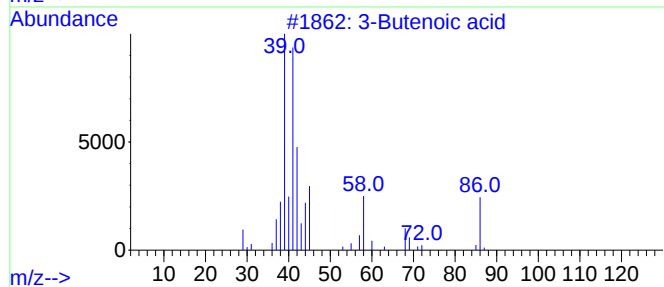
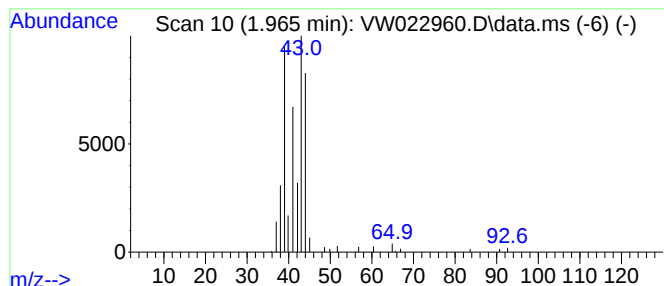
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM050222SMA.M
Quant Title : SFAM01.0

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

Peak Number 1 3-Butenoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.965	1.26 ug/L	26310	1,4-Difluorobenzene	8.842

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Butenoic acid	86	C4H6O2	000625-38-7	53
2			Cyclopropanecarboxamide	85	C4H7NO	006228-73-5	39
3			Chloro(prop-2-yn-1-yloxy)methanone	118	C4H3ClO2	035718-08-2	39
4			Propane	44	C3H8	000074-98-6	39
5			beta-Alanine amide	88	C3H8N2O	004726-85-6	9



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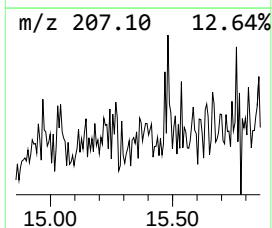
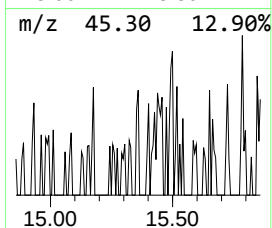
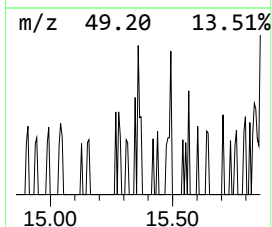
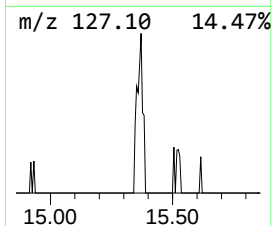
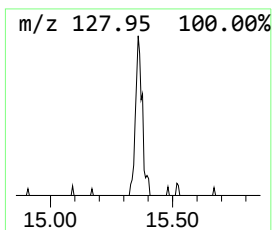
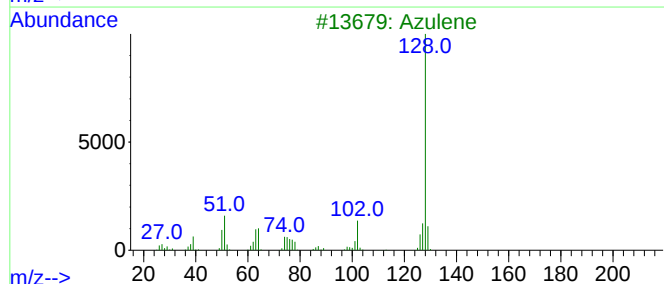
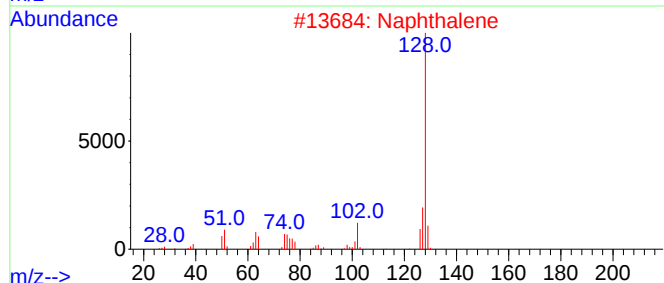
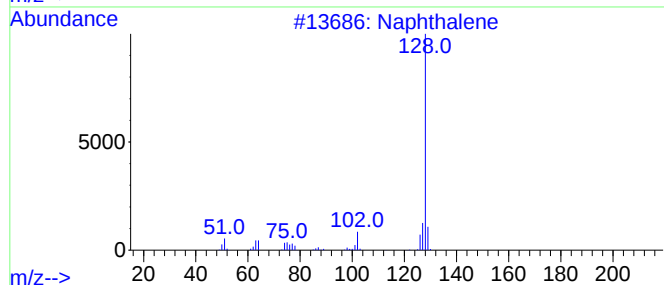
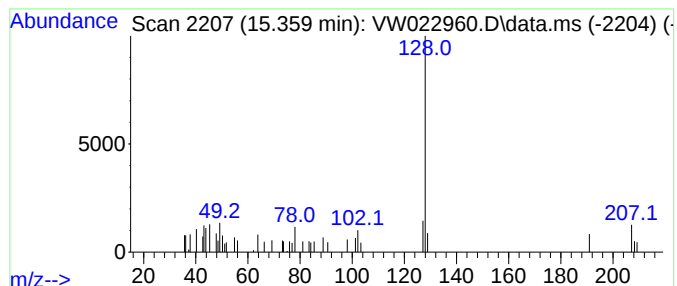
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.359	1.38 ug/L	5537	1,4-Dichlorobenzene-d4	13.560

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	59
2			Naphthalene	128	C10H8	000091-20-3	52
3			Azulene	128	C10H8	000275-51-4	52
4			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	50
5			Azulene	128	C10H8	000275-51-4	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Butenoic acid	1.965	1.3	ug/L	26310	1	8.842	520427	25.0
Azulene	15.359	1.4	ug/L	5537	3	13.560	100444	25.0