

Data Path : Z:\voasrv\HPCHEM1\MSVOA_W\Data\VW072524\
 Data File : VW029732.D
 Acq On : 25 Jul 2024 13:59
 Operator : SY/MD
 Sample : P3344-04
 Misc : 5.19g/10mL/MSVOA_W/SOIL/A
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_W
 ClientSampleId :
 BHB20

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\SFAMWLM072424SMA.M
 Title : SFAM01.0

Signal : TIC: VW029732.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.174	45	47	49	rBV	1097	859	0.07%	0.008%
2	2.369	71	79	97	rBV2	75364	216428	18.50%	2.110%
3	2.899	159	166	182	rVB2	34062	109689	9.37%	1.070%
4	3.393	245	247	252	rVV4	645	1037	0.09%	0.010%
5	3.564	273	275	282	rVB6	416	668	0.06%	0.007%
6	3.692	292	296	298	rBV4	729	1295	0.11%	0.013%
7	3.856	322	323	327	rVB4	652	781	0.07%	0.008%
8	4.021	339	350	363	rBV3	81863	274831	23.49%	2.680%
9	4.277	388	392	393	rBV3	793	1181	0.10%	0.012%
10	4.387	403	410	418	rBV2	3494	10834	0.93%	0.106%
11	4.490	425	427	432	rVB4	561	914	0.08%	0.009%
12	4.698	458	461	463	rBV2	537	645	0.06%	0.006%
13	4.771	471	473	477	rBV4	693	962	0.08%	0.009%
14	4.917	481	497	521	rBV	47823	198795	16.99%	1.939%
15	5.435	571	582	591	rVV4	10937	33692	2.88%	0.329%
16	5.679	619	622	624	rBV3	524	610	0.05%	0.006%
17	5.948	655	666	677	rBV4	4753	16247	1.39%	0.158%
18	6.082	685	688	691	rBV3	548	726	0.06%	0.007%
19	6.191	704	706	708	rVV3	728	689	0.06%	0.007%
20	6.216	708	710	712	rVV3	674	750	0.06%	0.007%
21	6.258	714	717	719	rVV4	652	644	0.06%	0.006%
22	6.588	768	771	777	rBV5	520	768	0.07%	0.007%
23	6.697	786	789	790	rVV3	574	654	0.06%	0.006%
24	6.911	815	824	831	rBV7	1621	5012	0.43%	0.049%
25	7.075	844	851	857	rBV	35218	94844	8.11%	0.925%
26	7.167	858	866	883	rVB	339311	913617	78.08%	8.909%
27	7.319	889	891	893	rVB3	698	624	0.05%	0.006%
28	7.551	922	929	932	rBV6	1217	2598	0.22%	0.025%
29	7.648	936	945	957	rVV	175449	436713	37.32%	4.259%
30	7.972	995	998	1002	rVB4	439	710	0.06%	0.007%
31	8.197	1032	1035	1038	rBV4	495	648	0.06%	0.006%
32	8.276	1038	1048	1066	rBV2	323023	990101	84.61%	9.655%
33	8.398	1066	1068	1071	rVV4	762	856	0.07%	0.008%
34	8.539	1089	1091	1093	rBV2	641	737	0.06%	0.007%
35	8.691	1111	1116	1117	rBV4	997	1317	0.11%	0.013%
36	8.843	1130	1141	1154	rBV	492721	980977	83.83%	9.566%

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 Title : SFAM01.0

37	9.093	1174	1182	1194	rVB2	24122	54390	4.65%	0.530%
38	9.270	1201	1211	1220	rBV	243631	503012	42.99%	4.905%
39	9.544	1254	1256	1262	rVB4	634	686	0.06%	0.007%
40	9.666	1269	1276	1281	rVV7	2004	4329	0.37%	0.042%
41	9.886	1308	1312	1313	rVV3	412	600	0.05%	0.006%
42	9.953	1319	1323	1324	rBV3	569	695	0.06%	0.007%
43	10.032	1327	1336	1347	rBV	117851	216896	18.54%	2.115%
44	10.130	1347	1352	1363	rVB	5993	13805	1.18%	0.135%
45	10.227	1366	1368	1370	rVB3	740	601	0.05%	0.006%
46	10.319	1374	1383	1390	rBV	419725	751210	64.20%	7.325%
47	10.386	1390	1394	1401	rVB	18834	31730	2.71%	0.309%
48	10.502	1408	1413	1419	rBV6	2461	5600	0.48%	0.055%
49	10.575	1419	1425	1435	rVV	77135	137662	11.76%	1.342%
50	10.697	1440	1445	1458	rVB	10602	24352	2.08%	0.237%
51	10.861	1466	1472	1476	rBV3	11488	19986	1.71%	0.195%
52	10.922	1476	1482	1491	rBV	137214	239305	20.45%	2.334%
53	11.075	1504	1507	1512	rVB4	4667	6866	0.59%	0.067%
54	11.142	1512	1518	1519	rBV6	1554	2542	0.22%	0.025%
55	11.190	1521	1526	1532	rBV6	4885	9430	0.81%	0.092%
56	11.270	1534	1539	1546	rVV3	5666	11575	0.99%	0.113%
57	11.404	1558	1561	1565	rVB6	3539	5164	0.44%	0.050%
58	11.507	1572	1578	1583	rBV6	10278	25187	2.15%	0.246%
59	11.629	1591	1598	1606	rBV	693553	1170149	100.00%	11.411%
60	11.709	1607	1611	1625	rVB	23843	49437	4.22%	0.482%
61	11.837	1627	1632	1633	rBV4	2623	3682	0.31%	0.036%
62	11.867	1635	1637	1649	rVB6	5684	10511	0.90%	0.102%
63	11.953	1649	1651	1654	rBV3	1311	1603	0.14%	0.016%
64	12.227	1694	1696	1697	rVV2	914	597	0.05%	0.006%
65	12.270	1701	1703	1707	rVV4	1373	1966	0.17%	0.019%
66	12.349	1711	1716	1719	rBV5	1162	2687	0.23%	0.026%
67	12.422	1727	1728	1734	rVB5	848	1165	0.10%	0.011%
68	12.520	1742	1744	1746	rVB3	1001	820	0.07%	0.008%
69	12.562	1746	1751	1753	rBV4	1358	2485	0.21%	0.024%
70	12.599	1753	1757	1764	rVB3	11006	17683	1.51%	0.172%
71	12.690	1764	1772	1779	rBV	199540	328856	28.10%	3.207%
72	12.812	1790	1792	1795	rVB4	654	714	0.06%	0.007%
73	12.879	1801	1803	1806	rBV3	871	1006	0.09%	0.010%
74	12.934	1809	1812	1813	rBV3	588	650	0.06%	0.006%
75	13.080	1834	1836	1838	rBV2	744	663	0.06%	0.006%
76	13.147	1842	1847	1850	rVB7	2077	3317	0.28%	0.032%

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 Title : SFAM01.0

77	13.202	1850	1856	1866	rBV3	4988	13965	1.19%	0.136%
78	13.324	1868	1876	1883	rVB3	2283	7501	0.64%	0.073%
79	13.391	1884	1887	1888	rBV3	1037	1038	0.09%	0.010%
80	13.458	1895	1898	1899	rBV2	913	779	0.07%	0.008%
81	13.477	1899	1901	1903	rVV2	1585	1950	0.17%	0.019%
82	13.501	1903	1905	1906	rVV2	1618	1483	0.13%	0.014%
83	13.556	1906	1914	1922	rVV	673376	1067129	91.20%	10.406%
84	13.647	1924	1929	1946	rVB2	19564	51837	4.43%	0.505%
85	13.849	1954	1962	1976	rBV	427538	708925	60.58%	6.913%
86	14.056	1992	1996	2003	rVB	10109	18065	1.54%	0.176%
87	14.184	2004	2017	2029	rVV7	24105	87491	7.48%	0.853%
88	14.318	2035	2039	2045	rVB6	4513	7196	0.61%	0.070%
89	14.464	2051	2063	2078	rBV2	91972	283863	24.26%	2.768%
90	14.714	2095	2104	2112	rBV10	4317	9767	0.83%	0.095%
91	15.086	2163	2165	2168	rBV4	1121	1784	0.15%	0.017%
92	15.178	2176	2180	2181	rBV3	1724	2337	0.20%	0.023%
93	15.391	2212	2215	2219	rVB4	1379	2105	0.18%	0.021%
94	15.476	2223	2229	2234	rVV	5105	9305	0.80%	0.091%
95	15.537	2236	2239	2247	rVB6	3467	5690	0.49%	0.055%
96	15.708	2262	2267	2268	rBV5	646	919	0.08%	0.009%
97	15.781	2275	2279	2282	rBV5	1884	3217	0.27%	0.031%
98	15.946	2304	2306	2307	rVV2	755	591	0.05%	0.006%
99	16.641	2418	2420	2423	rVV4	757	645	0.06%	0.006%
100	16.714	2430	2432	2437	rVB6	1083	1176	0.10%	0.011%

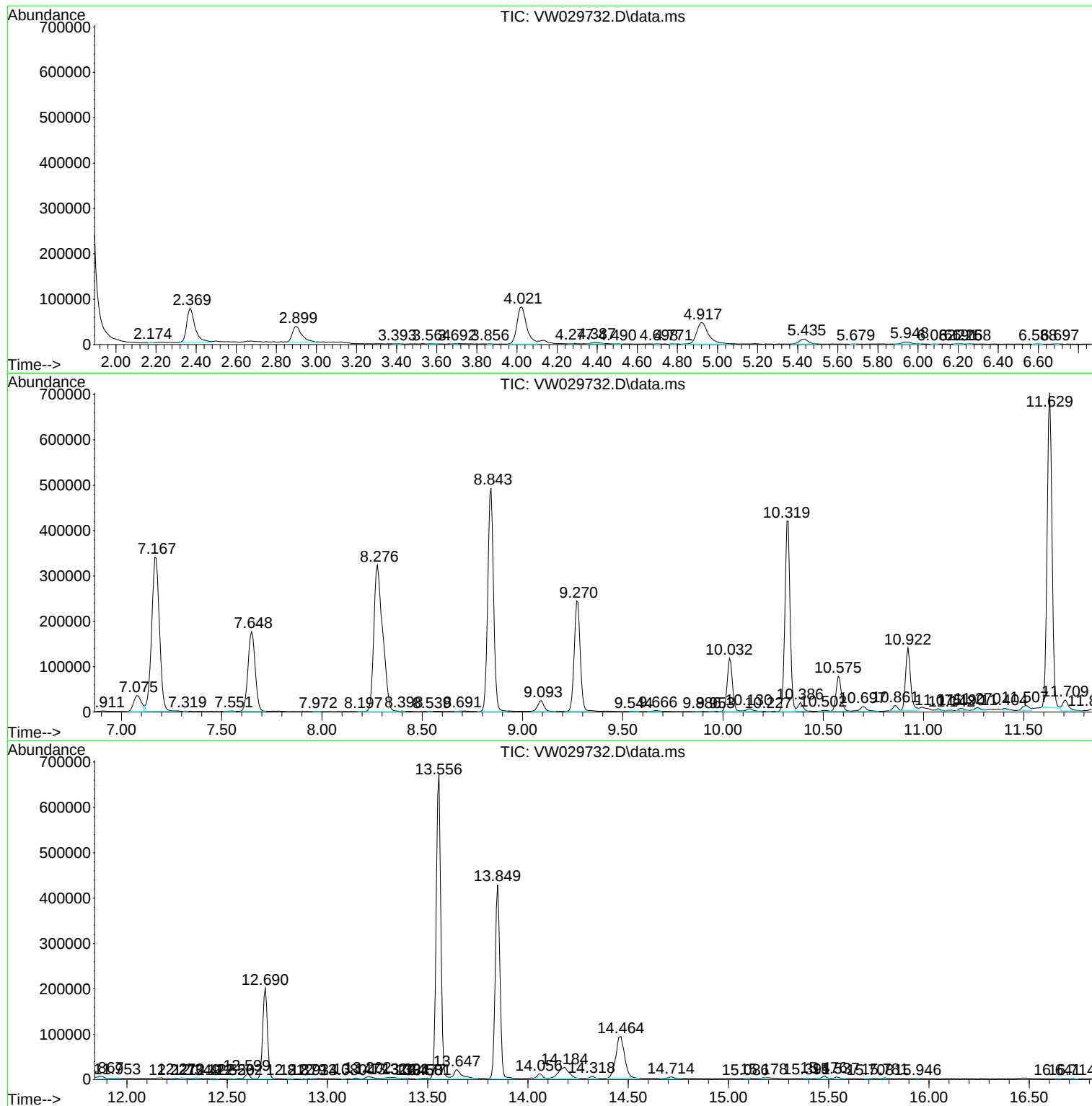
Sum of corrected areas: 10254825

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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



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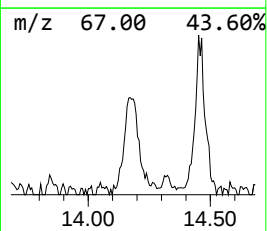
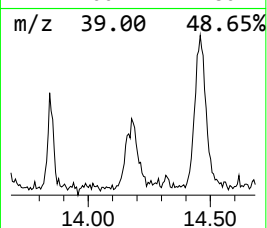
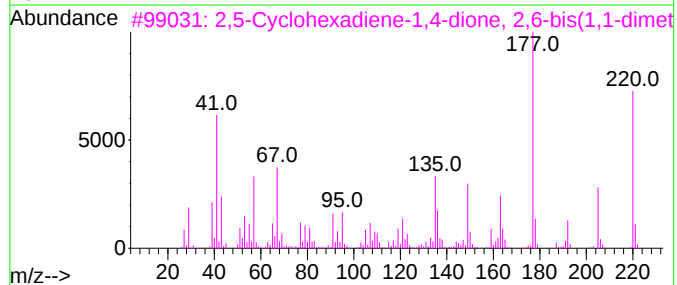
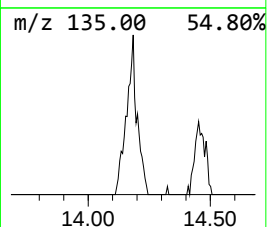
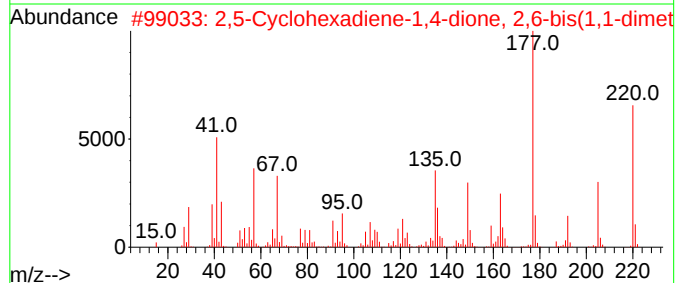
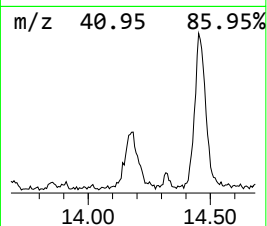
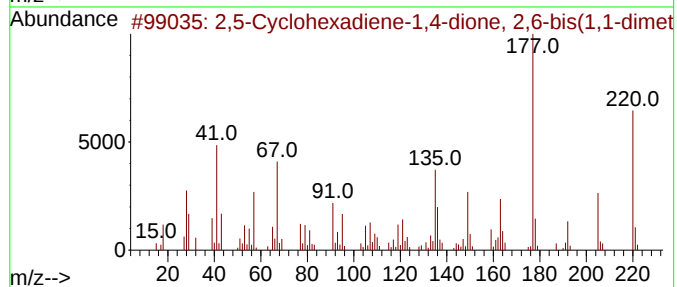
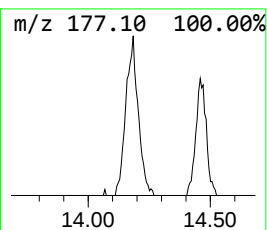
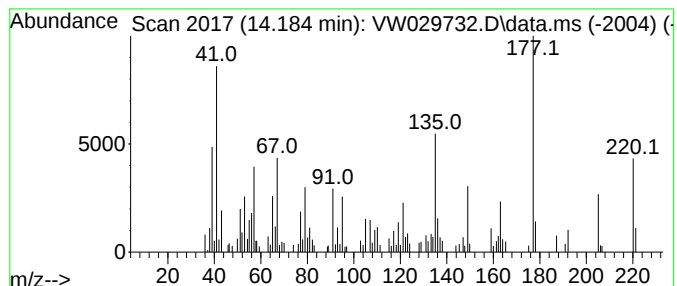
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 2 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.184	2.05 ug/L	87491	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	96
2			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	95
3			2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	87
4			Bicyclo[6.3.0]undec-1(8)-en-3-on...	220	C15H24O	1000164-02-7	64
5			.beta.-Oplophenone	220	C15H24O	028305-60-4	60



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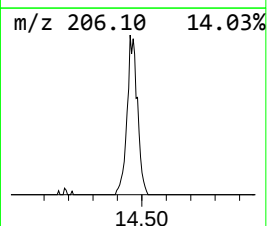
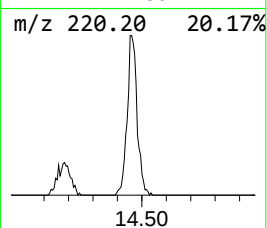
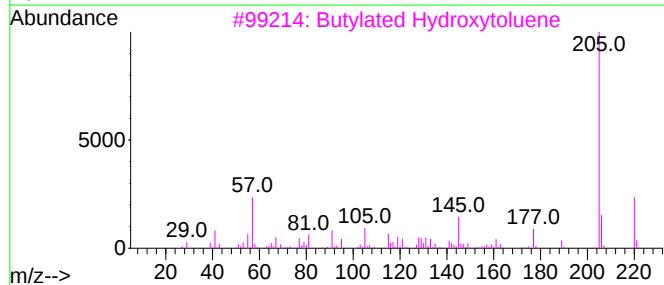
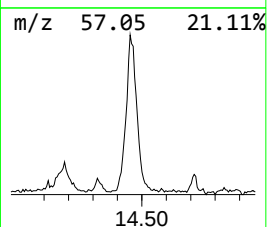
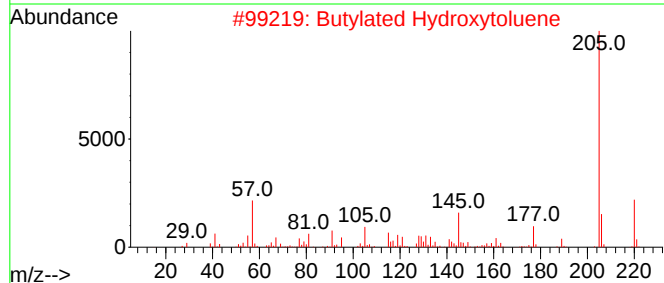
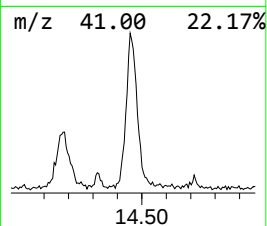
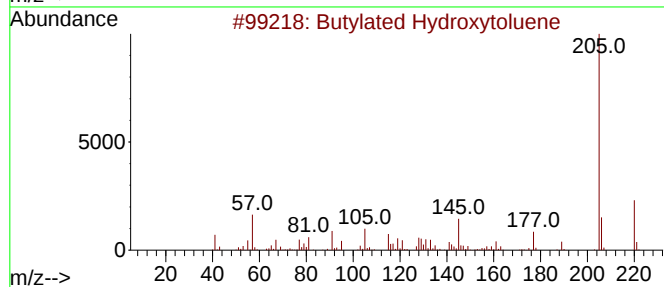
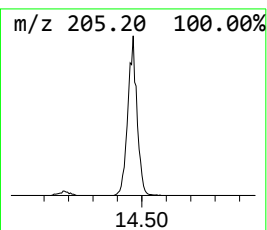
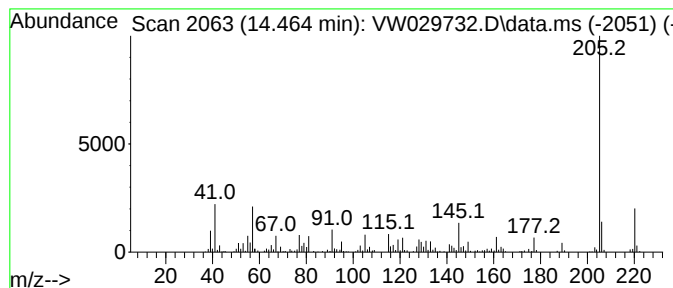
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_W\Method\SFAMWLM072424SMA.M
Quant Title : SFAM01.0

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

Peak Number 3 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.464	6.65 ug/L	283863	1,4-Dichlorobenzene-d4	13.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
2			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
3			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
4			Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	94
5			Butylated Hydroxytoluene	220	C15H24O	000128-37-0	93



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2,5-Cyclohexadi...	14.184	2.0	ug/L	87491	3	13.556	1067130	25.0
Butylated Hydro...	14.464	6.7	ug/L	283863	3	13.556	1067130	25.0