

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102518\
 Data File : VU027810.D
 Acq On : 25 Oct 2018 17:52
 Operator : MD/SY
 Sample : J5635-25ME 10X
 Misc : 4.91g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A40G1ME

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.399	64	70	81	rBV	40999	40791	13.07%	1.347%
2	1.672	147	155	172	rVB	29335	38700	12.40%	1.278%
3	2.270	331	341	355	rBV	63079	95280	30.53%	3.146%
4	2.479	403	406	409	rVB	205	146	0.05%	0.005%
5	2.617	446	449	456	rVB2	296	269	0.09%	0.009%
6	2.833	513	516	518	rBV2	313	228	0.07%	0.008%
7	3.247	639	645	649	rBV	224	331	0.11%	0.011%
8	3.443	702	706	712	rBV	182	290	0.09%	0.010%
9	3.923	850	855	859	rBV	149	209	0.07%	0.007%
10	3.974	869	871	876	rVB	172	163	0.05%	0.005%
11	4.032	882	889	894	rBV	190	363	0.12%	0.012%
12	4.180	922	935	959	rBV	30284	77272	24.76%	2.552%
13	4.337	979	984	988	rBV2	172	203	0.07%	0.007%
14	4.408	1003	1006	1011	rVB	202	181	0.06%	0.006%
15	4.443	1012	1017	1022	rBV	147	250	0.08%	0.008%
16	4.649	1065	1081	1105	rBV	53023	122189	39.15%	4.035%
17	4.759	1113	1115	1119	rVB	188	141	0.05%	0.005%
18	4.784	1119	1123	1124	rBV	157	134	0.04%	0.004%
19	4.810	1129	1131	1135	rBB	237	133	0.04%	0.004%
20	4.842	1136	1141	1144	rBV	295	315	0.10%	0.010%
21	4.903	1156	1160	1164	rVB2	256	277	0.09%	0.009%
22	5.074	1211	1213	1218	rVB	196	186	0.06%	0.006%
23	5.341	1272	1296	1313	rVV2	104641	312075	100.00%	10.306%
24	5.476	1335	1338	1340	rBV	161	137	0.04%	0.005%
25	5.540	1354	1358	1364	rBB	189	273	0.09%	0.009%
26	5.569	1365	1367	1370	rBV	180	150	0.05%	0.005%
27	5.755	1421	1425	1432	rBB	145	224	0.07%	0.007%
28	5.813	1440	1443	1445	rBV	162	130	0.04%	0.004%
29	5.887	1452	1466	1486	rBV	124287	241830	77.49%	7.986%
30	6.048	1513	1516	1518	rVB2	270	196	0.06%	0.006%
31	6.070	1519	1523	1526	rBB	157	127	0.04%	0.004%
32	6.090	1527	1529	1533	rBV	129	134	0.04%	0.004%
33	6.186	1556	1559	1561	rBV	164	131	0.04%	0.004%
34	6.228	1568	1572	1577	rBB	177	219	0.07%	0.007%

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 Title : VOC Analysis

35	6.331	1590	1604	1623	rBB2	74986	146114	46.82%	4.825%
36	6.549	1667	1672	1677	rBB	195	280	0.09%	0.009%
37	6.723	1723	1726	1731	rBV	158	215	0.07%	0.007%
38	6.791	1744	1747	1749	rBV	179	144	0.05%	0.005%
39	6.858	1761	1768	1778	rBV3	1237	2246	0.72%	0.074%
40	6.900	1778	1781	1784	rVB2	290	225	0.07%	0.007%
41	7.041	1823	1825	1828	rBV	152	124	0.04%	0.004%
42	7.061	1828	1831	1835	rVV	137	124	0.04%	0.004%
43	7.157	1858	1861	1864	rVB	185	145	0.05%	0.005%
44	7.228	1872	1883	1900	rBV	42945	74338	23.82%	2.455%
45	7.308	1906	1908	1914	rVB	183	202	0.06%	0.007%
46	7.344	1915	1919	1922	rBV	127	154	0.05%	0.005%
47	7.437	1945	1948	1953	rBV	167	213	0.07%	0.007%
48	7.566	1975	1988	2005	rVV	143728	242640	77.75%	8.013%
49	7.697	2024	2029	2031	rBV	164	178	0.06%	0.006%
50	7.778	2051	2054	2058	rBV	122	158	0.05%	0.005%
51	7.848	2065	2076	2097	rBV	30352	50115	16.06%	1.655%
52	7.964	2106	2112	2117	rBV2	262	397	0.13%	0.013%
53	8.003	2121	2124	2129	rVB2	199	178	0.06%	0.006%
54	8.183	2166	2180	2191	rBV	20565	49952	16.01%	1.650%
55	8.311	2211	2220	2247	rVB	111479	191111	61.24%	6.311%
56	8.620	2310	2316	2319	rBV	478	495	0.16%	0.016%
57	8.701	2336	2341	2343	rBV	149	150	0.05%	0.005%
58	8.819	2374	2378	2381	rVB2	269	262	0.08%	0.009%
59	8.852	2385	2388	2392	rVV	236	177	0.06%	0.006%
60	8.881	2393	2397	2403	rVV2	231	285	0.09%	0.009%
61	8.922	2407	2410	2412	rVV	171	127	0.04%	0.004%
62	8.948	2415	2418	2422	rVB2	287	239	0.08%	0.008%
63	8.977	2424	2427	2430	rBV2	253	185	0.06%	0.006%
64	9.090	2450	2462	2481	rVV	185394	302586	96.96%	9.992%
65	9.411	2560	2562	2566	rBV4	544	435	0.14%	0.014%
66	9.842	2693	2696	2698	rBV2	369	260	0.08%	0.009%
67	9.951	2724	2730	2735	rBV5	576	806	0.26%	0.027%
68	9.996	2741	2744	2750	rBV2	216	284	0.09%	0.009%
69	10.067	2764	2766	2770	rVB	205	164	0.05%	0.005%
70	10.093	2770	2774	2777	rBV	194	209	0.07%	0.007%
71	10.434	2868	2880	2897	rVB	96026	151721	48.62%	5.010%

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72	10.617	2924	2937	2950	rVB3	7422	15530	4.98%	0.513%
73	10.874	3012	3017	3026	rVB3	618	881	0.28%	0.029%
74	11.417	3183	3186	3188	rBV	253	144	0.05%	0.005%
75	11.482	3195	3206	3224	rBV	187586	298040	95.50%	9.842%
76	11.861	3312	3324	3341	rBV	144154	228266	73.14%	7.538%
77	11.951	3350	3352	3356	rVB	271	134	0.04%	0.004%
78	11.977	3356	3360	3363	rBV	157	127	0.04%	0.004%
79	12.308	3403	3463	3464	rBV7	27852	134522	43.11%	4.442%
80	12.617	3556	3559	3562	rBV2	264	178	0.06%	0.006%
81	12.646	3565	3568	3571	rBV3	284	221	0.07%	0.007%
82	13.170	3725	3731	3733	rBV3	422	418	0.13%	0.014%
83	14.195	4044	4050	4052	rBV4	766	759	0.24%	0.025%
84	14.276	4070	4075	4087	rVB2	5579	8776	2.81%	0.290%
85	14.421	4118	4120	4123	rBV	230	150	0.05%	0.005%
86	14.498	4141	4144	4151	rVB2	216	209	0.07%	0.007%
87	14.597	4151	4175	4177	rBV5	5067	12580	4.03%	0.415%
88	14.787	4230	4234	4241	rVB3	832	949	0.30%	0.031%
89	14.832	4241	4248	4255	rBV4	1815	2551	0.82%	0.084%
90	14.874	4257	4261	4265	rBV2	264	342	0.11%	0.011%
91	15.012	4299	4304	4312	rVB3	1117	1665	0.53%	0.055%
92	15.089	4322	4328	4338	rVB2	1473	1631	0.52%	0.054%
93	15.613	4485	4491	4501	rBV3	1854	3183	1.02%	0.105%
94	15.880	4564	4574	4583	rVB3	2497	4156	1.33%	0.137%
95	16.453	4749	4752	4758	rBV6	811	983	0.31%	0.032%
96	16.555	4774	4784	4794	rVB	96834	140384	44.98%	4.636%
97	16.623	4801	4805	4807	rBV2	670	583	0.19%	0.019%
98	16.707	4824	4831	4839	rVB3	4523	6455	2.07%	0.213%
99	16.903	4890	4892	4897	rBV2	545	438	0.14%	0.014%
100	17.488	5066	5074	5084	rVB5	7570	12581	4.03%	0.415%

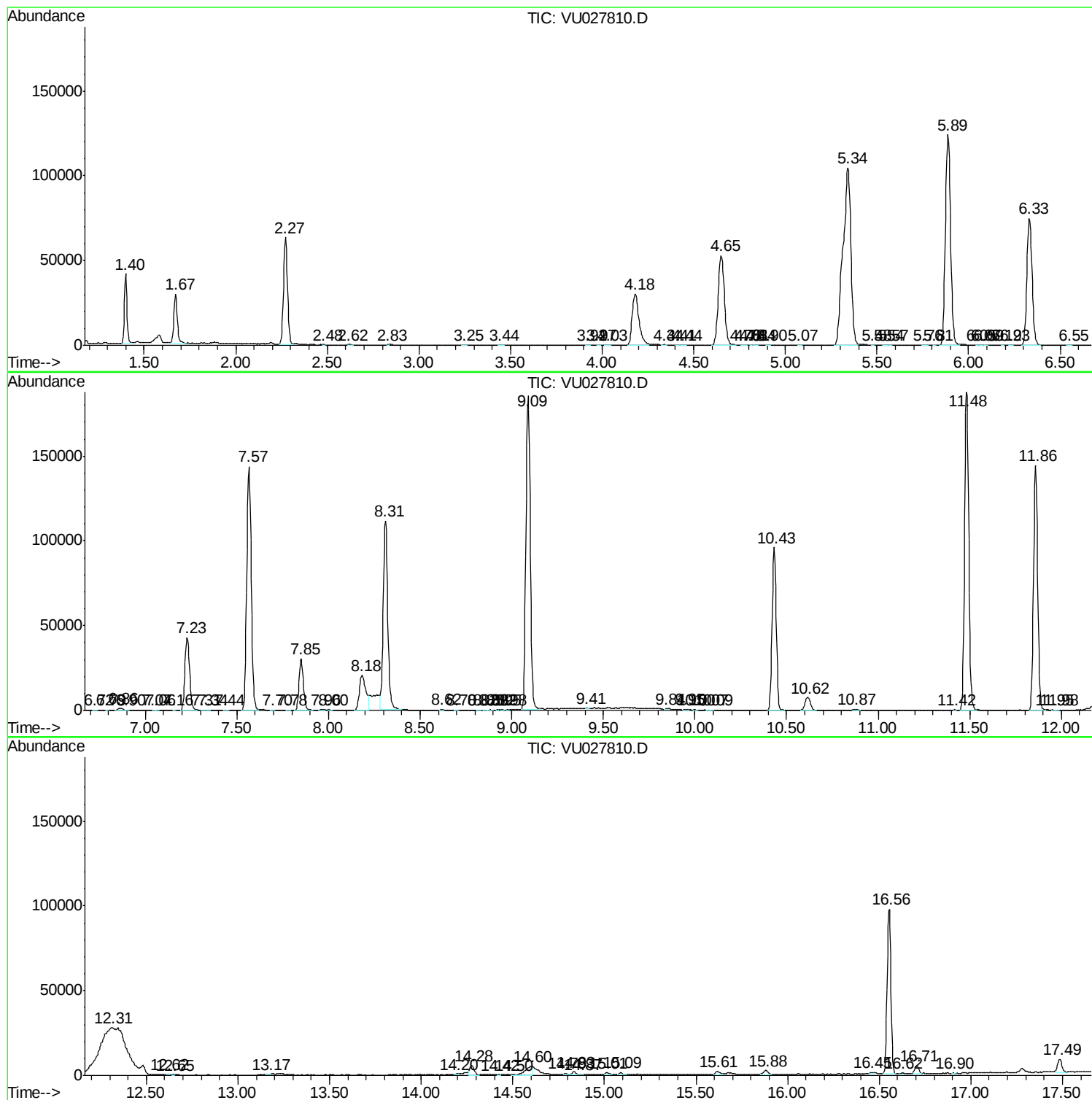
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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ALS Vial : 7 Sample Multiplier: 1

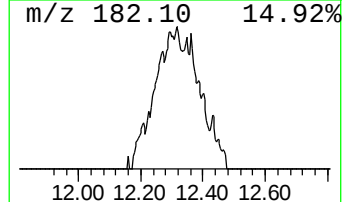
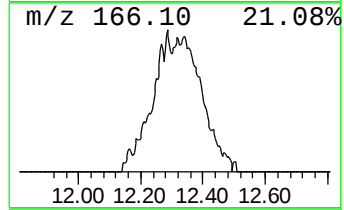
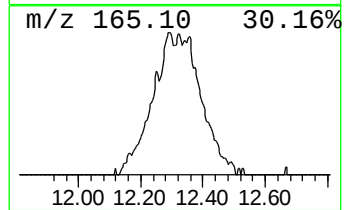
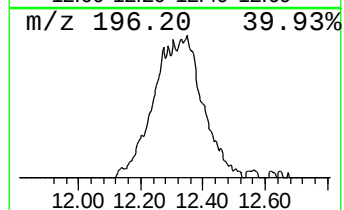
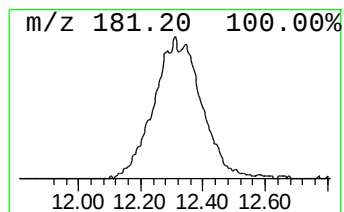
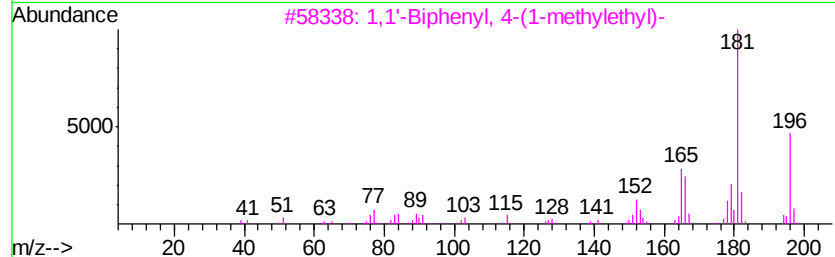
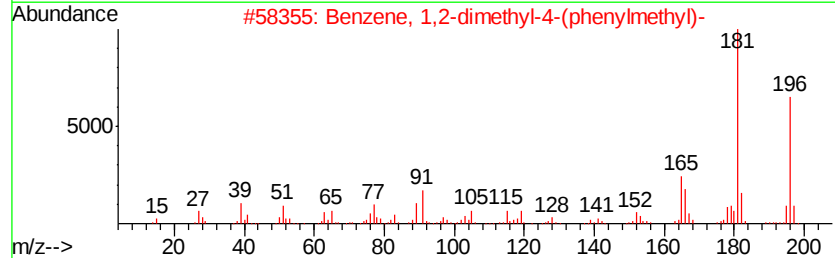
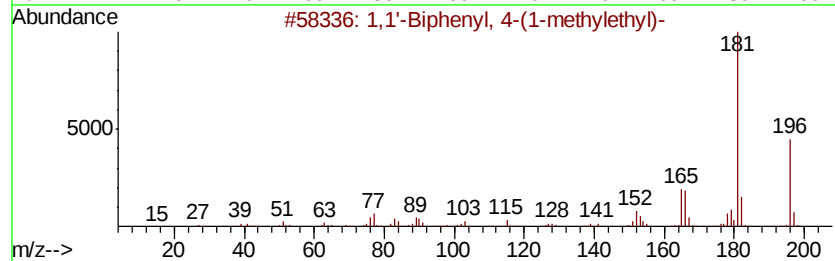
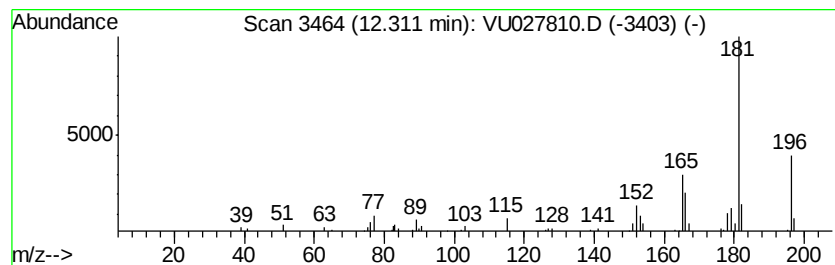
Instrument :
MSVOA_U
ClientSampleId :
A40G1ME

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1,1'-Biphenyl, 4-(1-methyle... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.31	22.57 ug/L	134522	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1,1'-Biphenyl, 4-(1-methylethyl)-	196 C15H16	007116-95-2 97
2		Benzene, 1,2-dimethyl-4-(phenylm...	196 C15H16	013540-56-2 94
3		1,1'-Biphenyl, 4-(1-methylethyl)-	196 C15H16	007116-95-2 94
4		1,1'-Biphenyl, 3-(1-methylethyl)-	196 C15H16	020282-30-8 93
5		9H-Carbazole, 2-methyl-	181 C13H11N	003652-91-3 91



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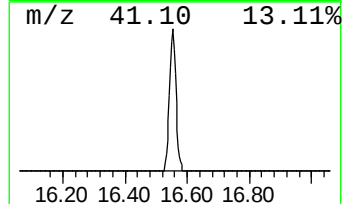
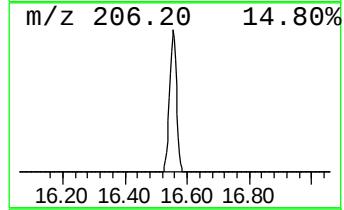
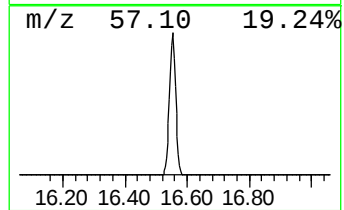
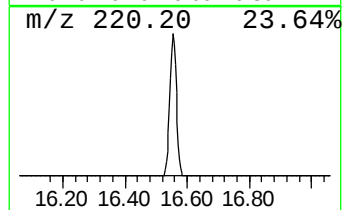
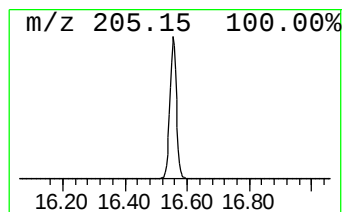
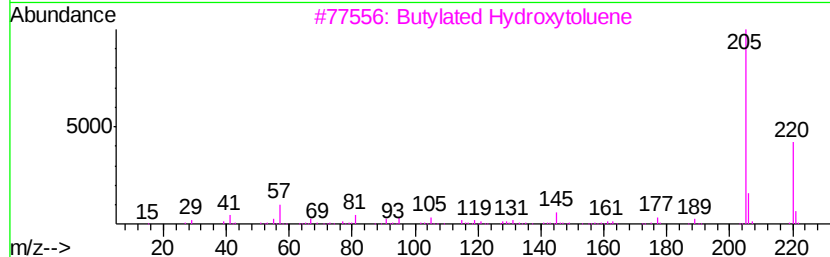
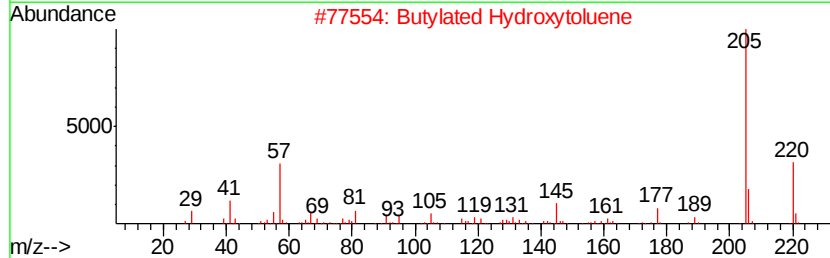
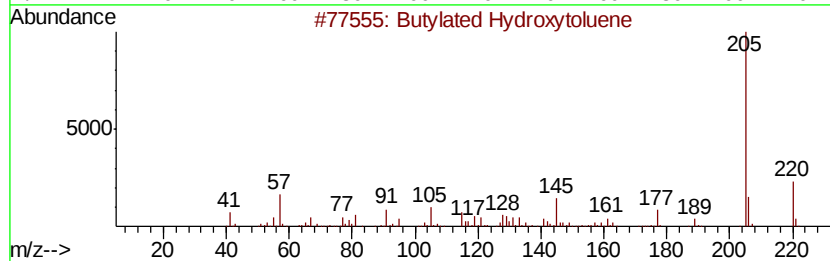
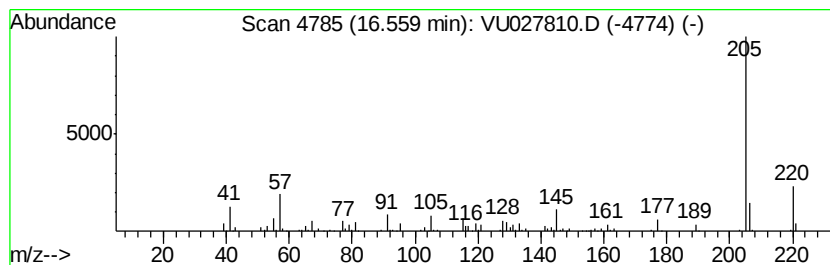
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.56	23.55 ug/L	140384	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	98
2		Butylated Hydroxytoluene	220	C15H24O	000128-37-0	96
3		Butylated Hydroxytoluene	220	C15H24O	000128-37-0	94
4		Butylated Hydroxytoluene	220	C15H24O	000128-37-0	93
5		Phenol, 2,4,6-tris(1-methylethyl)-	220	C15H24O	002934-07-8	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,1'-Biphenyl, 4-...	12.31	22.6	ug/L	134522	3	11.48	298040	50.0
Butylated Hydroxy...	16.56	23.6	ug/L	140384	3	11.48	298040	50.0