

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102518\
 Data File : VU027808.D
 Acq On : 25 Oct 2018 16:43
 Operator : MD/SY
 Sample : J5635-22ME 10X
 Misc : 4.83g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A40F8ME

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	63	70	83	rBV	40559	41669	13.55%	1.529%
2	1.669	146	154	167	rVB	28348	35369	11.51%	1.298%
3	1.881	215	220	229	rVB3	1007	1189	0.39%	0.044%
4	2.228	325	328	331	rBV2	550	398	0.13%	0.015%
5	2.270	331	341	355	rVV	62191	93176	30.31%	3.420%
6	2.350	364	366	371	rVB	257	159	0.05%	0.006%
7	2.472	401	404	410	rVB2	280	327	0.11%	0.012%
8	2.604	441	445	447	rBV	214	154	0.05%	0.006%
9	2.839	514	518	524	rVB	236	179	0.06%	0.007%
10	3.556	739	741	744	rBV	183	135	0.04%	0.005%
11	3.797	812	816	819	rBV	154	178	0.06%	0.007%
12	3.816	819	822	831	rVV2	288	298	0.10%	0.011%
13	3.868	836	838	846	rVB	328	334	0.11%	0.012%
14	3.910	847	851	854	rBV	197	216	0.07%	0.008%
15	3.958	863	866	869	rBV	141	141	0.05%	0.005%
16	3.987	871	875	879	rVB	111	134	0.04%	0.005%
17	4.099	907	910	913	rBV	170	165	0.05%	0.006%
18	4.177	920	934	959	rBV	28481	71051	23.11%	2.608%
19	4.308	972	975	978	rBV	167	152	0.05%	0.006%
20	4.649	1065	1081	1103	rBV	51372	121066	39.38%	4.443%
21	4.833	1135	1138	1141	rBV2	280	241	0.08%	0.009%
22	4.874	1149	1151	1156	rVB2	147	153	0.05%	0.006%
23	4.926	1163	1167	1169	rBV	162	156	0.05%	0.006%
24	4.958	1174	1177	1181	rVB	263	169	0.05%	0.006%
25	5.138	1230	1233	1235	rBV	167	140	0.05%	0.005%
26	5.341	1272	1296	1323	rBV2	103320	307421	100.00%	11.283%
27	5.466	1329	1335	1340	rBV	144	265	0.09%	0.010%
28	5.572	1363	1368	1371	rBV	141	191	0.06%	0.007%
29	5.630	1379	1386	1390	rBB	170	240	0.08%	0.009%
30	5.652	1391	1393	1397	rBV	153	148	0.05%	0.005%
31	5.733	1416	1418	1422	rBV	174	184	0.06%	0.007%
32	5.887	1453	1466	1482	rBV	121397	234471	76.27%	8.606%
33	6.019	1504	1507	1510	rVB	189	152	0.05%	0.006%
34	6.122	1534	1539	1541	rBV	167	188	0.06%	0.007%

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Integration Parameters: LSCINT.P

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

35	6.263	1580	1583	1585	rBV	161	139	0.05%	0.005%
36	6.331	1591	1604	1624	rVB2	73107	143620	46.72%	5.271%
37	6.453	1637	1642	1644	rBV	206	187	0.06%	0.007%
38	6.537	1664	1668	1670	rBV	166	168	0.05%	0.006%
39	6.588	1680	1684	1687	rBV	163	178	0.06%	0.007%
40	6.787	1742	1746	1750	rBB	161	191	0.06%	0.007%
41	6.813	1751	1754	1756	rBV	162	128	0.04%	0.005%
42	6.829	1756	1759	1762	rVV	141	130	0.04%	0.005%
43	6.861	1762	1769	1781	rVB4	1125	2100	0.68%	0.077%
44	6.974	1801	1804	1810	rBB	194	229	0.07%	0.008%
45	7.106	1840	1845	1846	rBV	146	147	0.05%	0.005%
46	7.228	1872	1883	1901	rVV2	41583	73059	23.77%	2.681%
47	7.566	1976	1988	2010	rVV	138236	236041	76.78%	8.663%
48	7.646	2012	2013	2018	rVV	404	149	0.05%	0.005%
49	7.729	2036	2039	2048	rVB	178	304	0.10%	0.011%
50	7.768	2048	2051	2054	rBV	169	161	0.05%	0.006%
51	7.848	2067	2076	2090	rBV	28877	47486	15.45%	1.743%
52	8.183	2167	2180	2188	rBV2	12172	26795	8.72%	0.983%
53	8.311	2211	2220	2249	rVB	106836	178365	58.02%	6.546%
54	8.620	2314	2316	2319	rVB	403	265	0.09%	0.010%
55	8.639	2319	2322	2325	rBV	162	165	0.05%	0.006%
56	8.720	2344	2347	2351	rBB	168	159	0.05%	0.006%
57	8.752	2354	2357	2359	rBV	213	174	0.06%	0.006%
58	8.816	2373	2377	2382	rVB	183	242	0.08%	0.009%
59	8.848	2383	2387	2396	rBB	193	359	0.12%	0.013%
60	8.890	2396	2400	2403	rBB	171	161	0.05%	0.006%
61	8.910	2403	2406	2408	rBV	173	139	0.05%	0.005%
62	8.967	2420	2424	2428	rBV	191	243	0.08%	0.009%
63	9.090	2449	2462	2488	rBV	179822	292407	95.12%	10.732%
64	9.266	2512	2517	2525	rBV	185	352	0.11%	0.013%
65	9.620	2624	2627	2630	rBV	167	173	0.06%	0.006%
66	9.948	2726	2729	2736	rBV3	500	627	0.20%	0.023%
67	10.176	2794	2800	2803	rBV	173	159	0.05%	0.006%
68	10.434	2868	2880	2897	rVV	94879	149412	48.60%	5.484%
69	10.498	2897	2900	2904	rVB	222	201	0.07%	0.007%
70	10.543	2909	2914	2919	rBV	213	309	0.10%	0.011%
71	10.614	2925	2936	2952	rVB4	5607	11149	3.63%	0.409%

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 Title : VOC Analysis

72	10.871	3010	3016	3019	rBV	478	515	0.17%	0.019%
73	11.424	3185	3188	3195	rBV2	420	285	0.09%	0.010%
74	11.485	3195	3207	3229	rVV	179912	283962	92.37%	10.422%
75	11.771	3292	3296	3300	rBV	146	161	0.05%	0.006%
76	11.861	3312	3324	3343	rBV	139938	223366	72.66%	8.198%
77	12.485	3505	3518	3526	rBV3	2031	3700	1.20%	0.136%
78	12.655	3568	3571	3575	rBV	203	157	0.05%	0.006%
79	13.758	3910	3914	3920	rBV2	326	284	0.09%	0.010%
80	14.276	4066	4075	4086	rBV2	2842	4780	1.55%	0.175%
81	14.459	4130	4132	4137	rVB2	166	142	0.05%	0.005%
82	14.552	4157	4161	4164	rBV	205	152	0.05%	0.006%
83	14.572	4164	4167	4171	rBV	159	164	0.05%	0.006%
84	14.610	4176	4179	4182	rVB	304	188	0.06%	0.007%
85	14.768	4224	4228	4229	rBV	182	143	0.05%	0.005%
86	14.787	4229	4234	4239	rVV3	1467	1479	0.48%	0.054%
87	14.832	4241	4248	4259	rVB3	2236	3430	1.12%	0.126%
88	14.887	4260	4265	4268	rBV2	313	317	0.10%	0.012%
89	15.015	4296	4305	4315	rVB5	2137	3515	1.14%	0.129%
90	15.057	4315	4318	4322	rBV	194	186	0.06%	0.007%
91	15.093	4322	4329	4337	rVB4	1605	2183	0.71%	0.080%
92	15.183	4355	4357	4367	rVB3	681	587	0.19%	0.022%
93	15.613	4483	4491	4504	rBV2	3872	6175	2.01%	0.227%
94	15.884	4568	4575	4584	rVB2	1801	2559	0.83%	0.094%
95	16.478	4756	4760	4765	rBV3	749	817	0.27%	0.030%
96	16.556	4773	4784	4795	rBV2	46310	67553	21.97%	2.479%
97	16.703	4824	4830	4838	rVB2	4843	6312	2.05%	0.232%
98	17.199	4981	4984	4985	rBV3	605	305	0.10%	0.011%
99	17.279	5003	5009	5018	rVB2	5830	7458	2.43%	0.274%
100	17.488	5064	5074	5085	rVB4	15839	26888	8.75%	0.987%

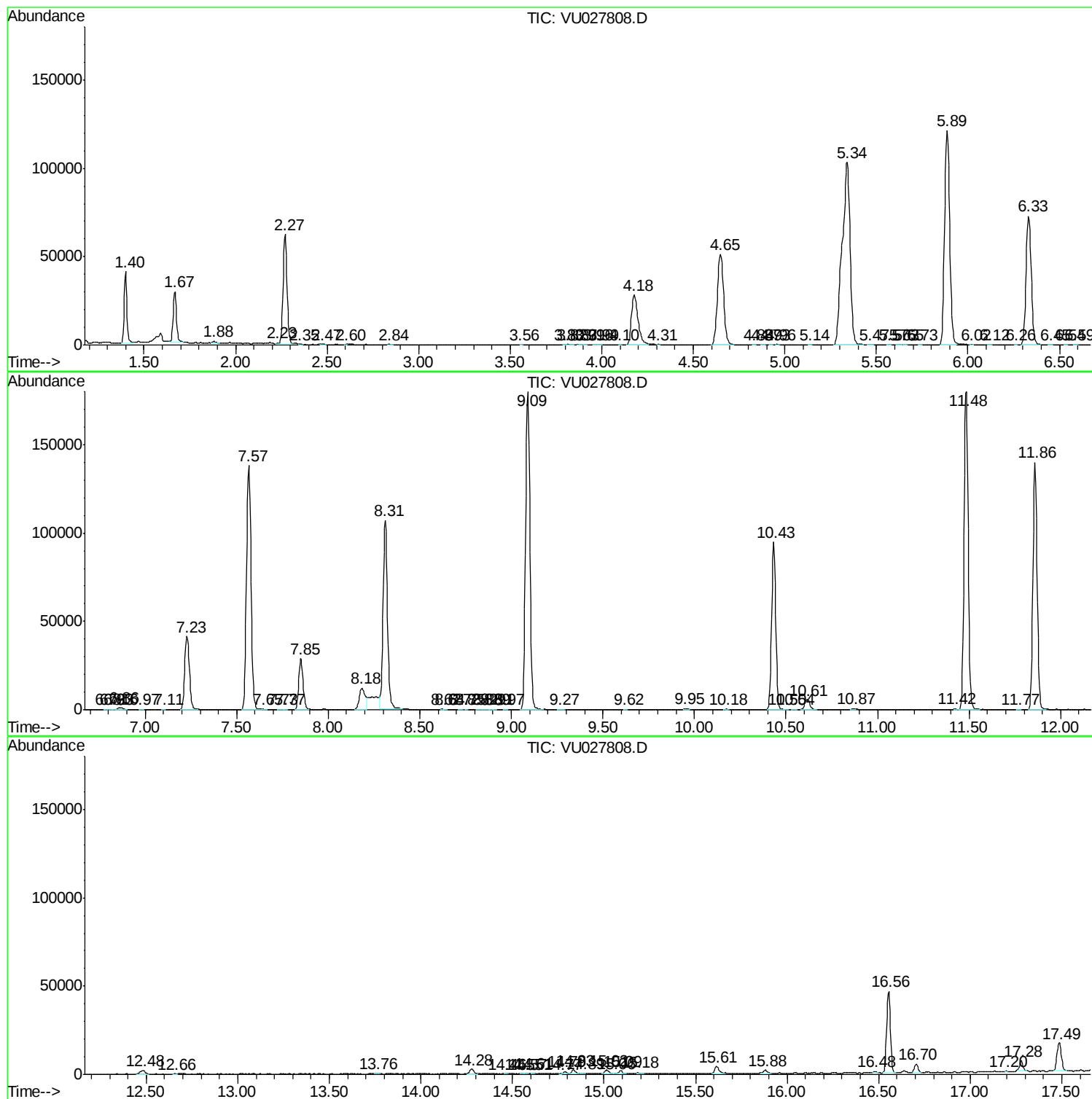
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 4 Sample Multiplier: 1

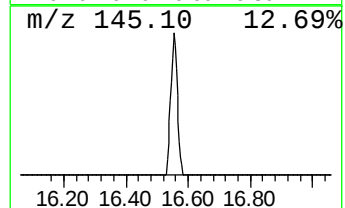
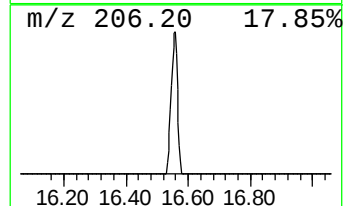
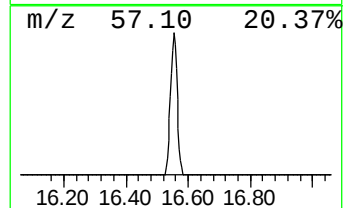
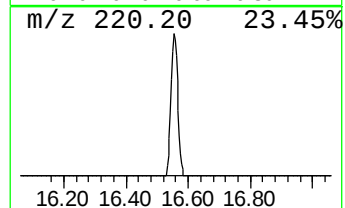
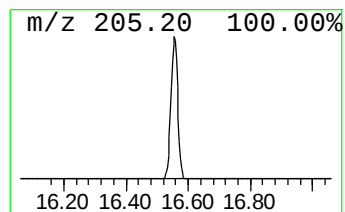
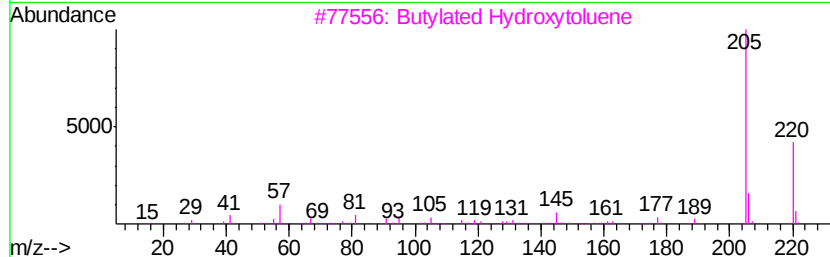
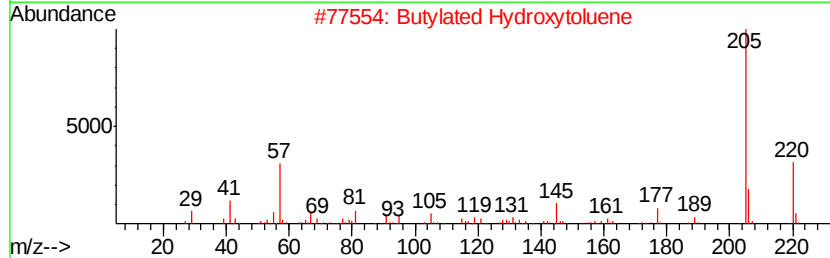
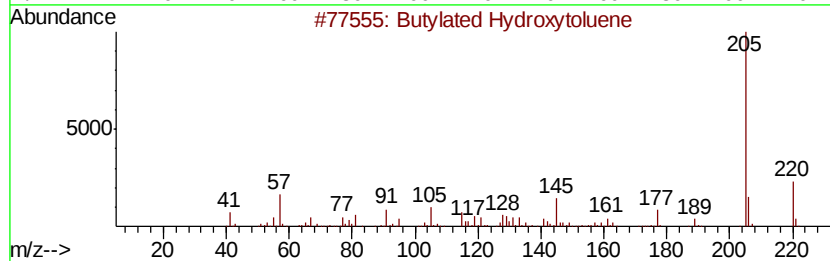
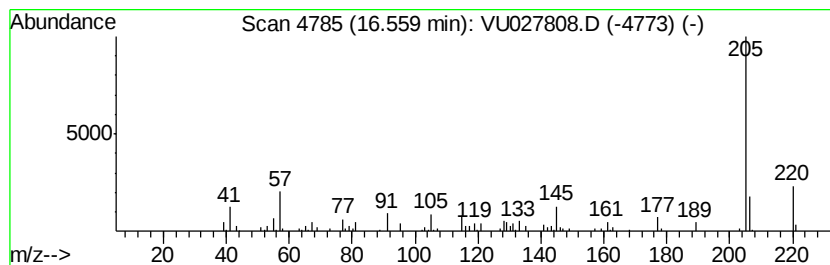
Instrument :
MSVOA_U
ClientSampleId :
A40F8ME

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 3 Butylated Hydroxytoluene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.56	11.89 ug/L	67553	1,4-Dichlorobenzene-d4	11.48		
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	97
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	83



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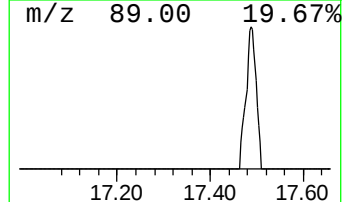
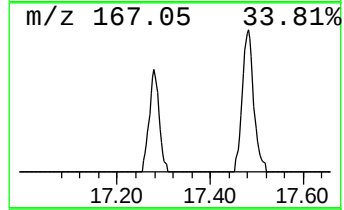
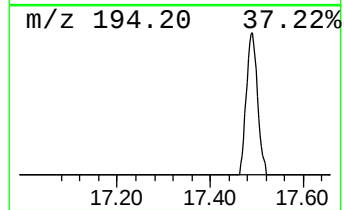
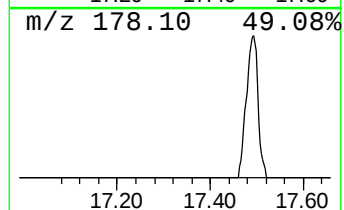
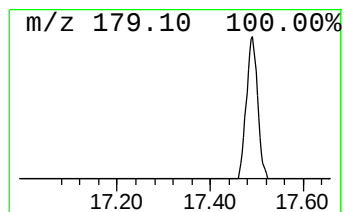
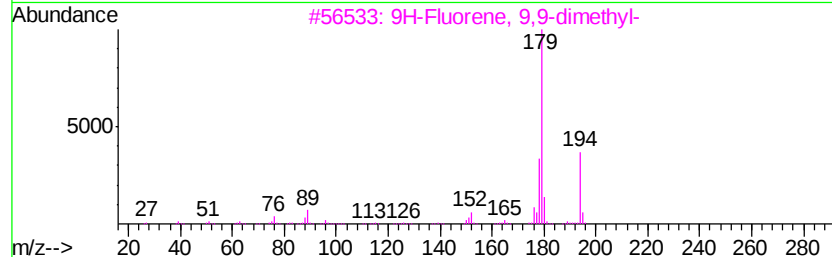
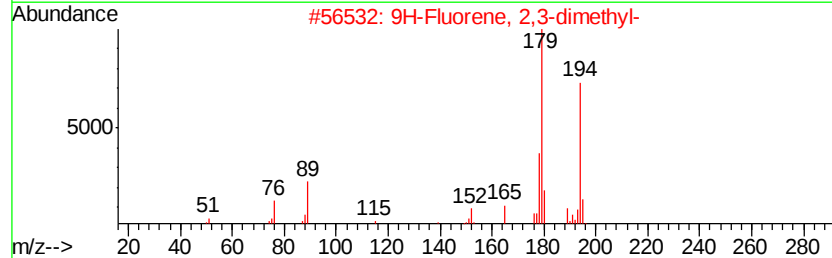
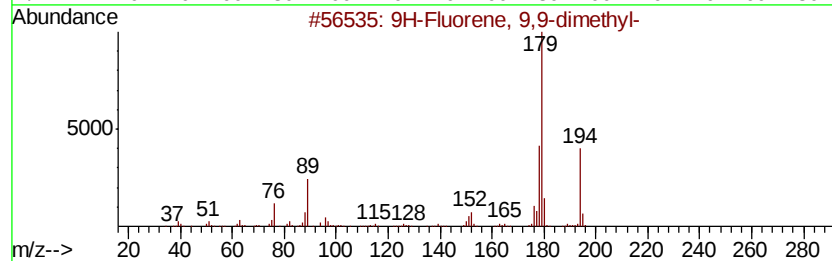
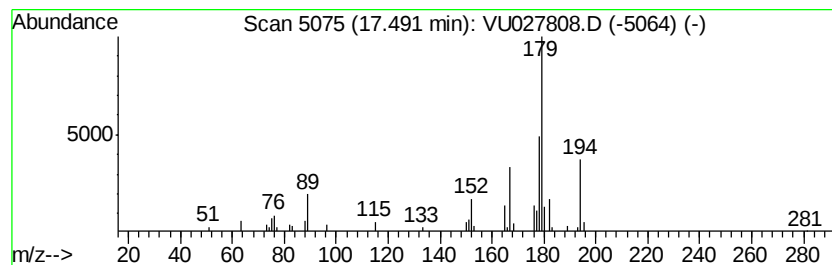
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Quant Title : VOC Analysis

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

Peak Number 4 9H-Fluorene, 9,9-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.49	4.73 ug/L	26888	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9H-Fluorene, 9,9-dimethyl-	194	C15H14	004569-45-3	95
2		9H-Fluorene, 2,3-dimethyl-	194	C15H14	004612-63-9	70
3		9H-Fluorene, 9,9-dimethyl-	194	C15H14	004569-45-3	70
4		1,1'-Biphenyl, 2-(1-azido-1-meth...	237	C15H15N3	032366-24-8	53
5		Phenanthro[1,2-c]furan-1,3-dione...	252	C16H12O3	063084-72-0	50



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butylated Hydroxy...	16.56	11.9	ug/L	67553	3	11.48	283962	50.0
9H-Fluorene, 9,9-...	17.49	4.7	ug/L	26888	3	11.48	283962	50.0