

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102518\
 Data File : VU027813.D
 Acq On : 25 Oct 2018 20:49
 Operator : MD/SY
 Sample : J5657-01MEDL 100X
 Misc : 4.65µ/5mL/100µL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A40G4MEDL

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	1.398	63	70	81	rBV	42610	43363	13.31%	1.395%
2	1.562	116	121	125	rVB4	1820	1936	0.59%	0.062%
3	1.681	150	158	172	rVB	30671	40600	12.46%	1.306%
4	2.273	332	342	355	rBV	65090	99436	30.52%	3.199%
5	2.450	391	397	400	rBV2	254	276	0.08%	0.009%
6	2.617	443	449	455	rBV2	247	289	0.09%	0.009%
7	2.704	470	476	485	rBV3	1218	1727	0.53%	0.056%
8	3.009	566	571	575	rBV	118	122	0.04%	0.004%
9	3.160	615	618	623	rBV	212	244	0.07%	0.008%
10	3.392	684	690	692	rBV	172	239	0.07%	0.008%
11	3.736	794	797	800	rBV	175	176	0.05%	0.006%
12	3.858	832	835	838	rVB	182	144	0.04%	0.005%
13	3.884	841	843	846	rBV	178	131	0.04%	0.004%
14	3.922	850	855	858	rBV	148	198	0.06%	0.006%
15	4.003	876	880	884	rBV	149	206	0.06%	0.007%
16	4.180	920	935	971	rBV	31654	84308	25.87%	2.712%
17	4.395	997	1002	1007	rBB	182	232	0.07%	0.007%
18	4.424	1007	1011	1013	rBV	164	158	0.05%	0.005%
19	4.556	1049	1052	1055	rVB	155	126	0.04%	0.004%
20	4.582	1055	1060	1065	rBV	229	315	0.10%	0.010%
21	4.652	1065	1082	1102	rBV2	54225	127842	39.23%	4.113%
22	4.855	1142	1145	1147	rVB2	247	136	0.04%	0.004%
23	4.871	1148	1150	1151	rBV	229	130	0.04%	0.004%
24	4.906	1159	1161	1165	rBV	247	220	0.07%	0.007%
25	4.929	1165	1168	1172	rVB	185	177	0.05%	0.006%
26	4.964	1175	1179	1181	rBV	143	151	0.05%	0.005%
27	5.025	1195	1198	1201	rVB	163	129	0.04%	0.004%
28	5.173	1238	1244	1247	rBB	142	193	0.06%	0.006%
29	5.344	1274	1297	1321	rBV2	108624	325855	100.00%	10.483%
30	5.450	1325	1330	1338	rVB2	290	460	0.14%	0.015%
31	5.498	1342	1345	1352	rBB	157	234	0.07%	0.008%
32	5.582	1366	1371	1373	rBV	185	206	0.06%	0.007%
33	5.617	1379	1382	1386	rBB	182	165	0.05%	0.005%
34	5.659	1390	1395	1399	rBB	194	224	0.07%	0.007%

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 Title : VOC Analysis

35	5.733	1416	1418	1422	rBV	129	144	0.04%	0.005%
36	5.887	1453	1466	1490	rBV	129647	255179	78.31%	8.210%
37	5.971	1490	1492	1500	rVV2	130	185	0.06%	0.006%
38	6.180	1553	1557	1562	rBB2	371	319	0.10%	0.010%
39	6.212	1563	1567	1570	rBV	175	191	0.06%	0.006%
40	6.260	1577	1582	1586	rBV	139	214	0.07%	0.007%
41	6.331	1592	1604	1624	rBV	76496	151941	46.63%	4.888%
42	6.559	1670	1675	1680	rBV	175	269	0.08%	0.009%
43	6.765	1733	1739	1745	rBB	143	241	0.07%	0.008%
44	6.832	1755	1760	1762	rBV	174	196	0.06%	0.006%
45	6.858	1762	1768	1779	rVB4	1100	2106	0.65%	0.068%
46	6.961	1797	1800	1807	rBB	200	283	0.09%	0.009%
47	7.009	1812	1815	1818	rBV	142	145	0.04%	0.005%
48	7.041	1822	1825	1827	rBV	147	124	0.04%	0.004%
49	7.170	1861	1865	1867	rBV	160	158	0.05%	0.005%
50	7.228	1872	1883	1901	rVV2	43996	77562	23.80%	2.495%
51	7.295	1901	1904	1907	rVB	266	185	0.06%	0.006%
52	7.417	1937	1942	1945	rBV	169	225	0.07%	0.007%
53	7.565	1976	1988	2010	rVV	146449	251517	77.19%	8.092%
54	7.852	2066	2077	2093	rVV	30773	51985	15.95%	1.672%
55	8.183	2168	2180	2190	rBV3	22157	49467	15.18%	1.591%
56	8.311	2211	2220	2245	rVB	112817	193794	59.47%	6.235%
57	8.588	2302	2306	2308	rVV2	230	139	0.04%	0.004%
58	8.617	2308	2315	2324	rVV2	1139	1601	0.49%	0.052%
59	8.742	2351	2354	2356	rBV	178	144	0.04%	0.005%
60	8.823	2377	2379	2382	rBV3	265	198	0.06%	0.006%
61	9.089	2450	2462	2477	rBV	196511	318628	97.78%	10.251%
62	10.109	2776	2779	2782	rVB	274	149	0.05%	0.005%
63	10.131	2782	2786	2787	rBV	166	121	0.04%	0.004%
64	10.183	2798	2802	2805	rBV	172	209	0.06%	0.007%
65	10.430	2867	2879	2899	rVB	99510	156232	47.95%	5.026%
66	10.568	2919	2922	2926	rVV	159	130	0.04%	0.004%
67	10.610	2926	2935	2951	rVB3	8910	16664	5.11%	0.536%
68	10.877	3010	3018	3026	rVB2	671	1128	0.35%	0.036%
69	10.916	3027	3030	3035	rBV	103	121	0.04%	0.004%
70	11.421	3182	3187	3192	rVB2	281	275	0.08%	0.009%
71	11.482	3195	3206	3223	rBV	198498	312801	95.99%	10.063%

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72	11.575	3231	3235	3238	rBV2	165	137	0.04%	0.004%
73	11.861	3311	3324	3339	rBV	143860	233664	71.71%	7.517%
74	12.183	3403	3424	3425	rBV6	6729	11337	3.48%	0.365%
75	12.617	3556	3559	3561	rBV2	326	256	0.08%	0.008%
76	12.694	3579	3583	3584	rBV	229	134	0.04%	0.004%
77	12.742	3594	3598	3603	rVB	239	242	0.07%	0.008%
78	12.793	3611	3614	3618	rVB	220	142	0.04%	0.005%
79	12.845	3626	3630	3635	rVB	206	169	0.05%	0.005%
80	13.137	3715	3721	3724	rBV2	288	271	0.08%	0.009%
81	13.163	3724	3729	3731	rBV2	417	372	0.11%	0.012%
82	13.411	3802	3806	3808	rBV2	210	168	0.05%	0.005%
83	14.176	4041	4044	4045	rBV	464	261	0.08%	0.008%
84	14.202	4048	4052	4053	rBV	843	568	0.17%	0.018%
85	14.327	4088	4091	4095	rVB2	298	189	0.06%	0.006%
86	14.353	4095	4099	4101	rBV2	462	333	0.10%	0.011%
87	14.414	4115	4118	4123	rBV	232	213	0.07%	0.007%
88	14.588	4147	4172	4205	rBV6	14788	69106	21.21%	2.223%
89	14.829	4243	4247	4258	rVB5	1760	2044	0.63%	0.066%
90	14.938	4278	4281	4284	rBV2	313	223	0.07%	0.007%
91	15.012	4297	4304	4311	rBV5	1378	1944	0.60%	0.063%
92	15.060	4312	4319	4324	rBV3	2184	2631	0.81%	0.085%
93	15.617	4489	4492	4496	rBV2	538	387	0.12%	0.012%
94	15.665	4505	4507	4508	rBV2	879	372	0.11%	0.012%
95	15.880	4566	4574	4584	rVB2	2441	4120	1.26%	0.133%
96	16.452	4741	4752	4760	rBV8	4869	11522	3.54%	0.371%
97	16.552	4773	4783	4800	rVB	117998	172901	53.06%	5.563%
98	16.613	4800	4802	4807	rVB2	545	467	0.14%	0.015%
99	16.703	4822	4830	4840	rVB3	10551	15223	4.67%	0.490%
100	17.276	5002	5008	5023	rBV4	1812	3580	1.10%	0.115%

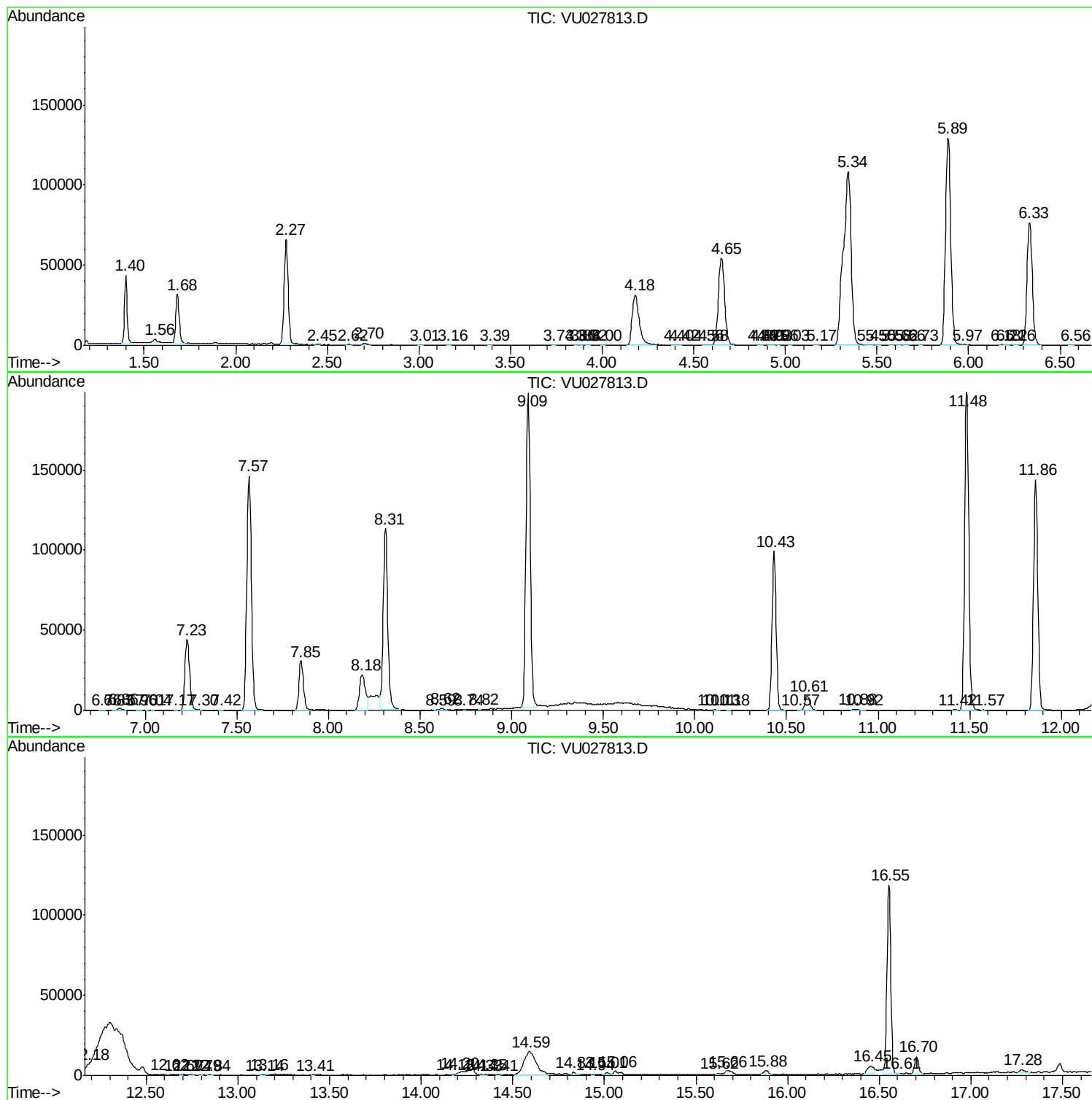
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Instrument :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

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



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A40G4MEDL

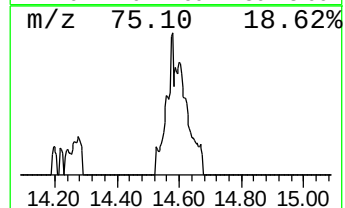
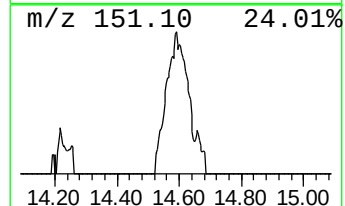
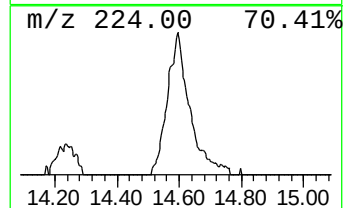
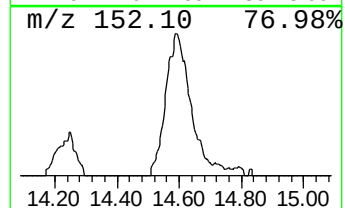
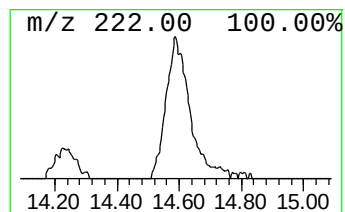
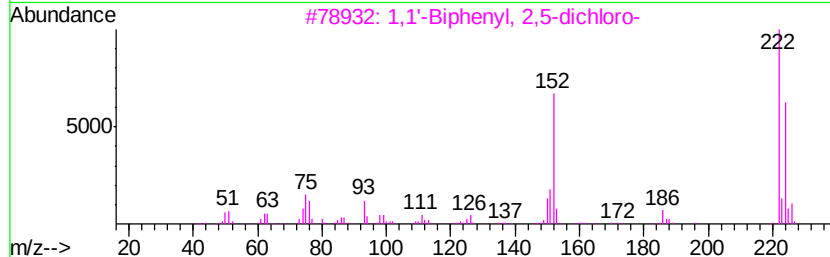
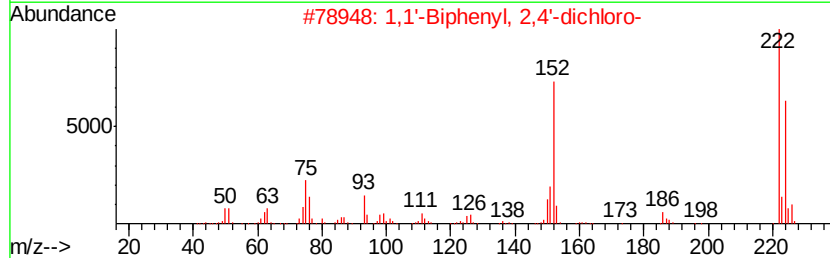
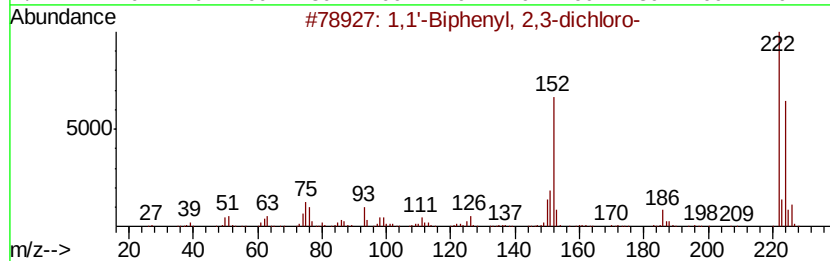
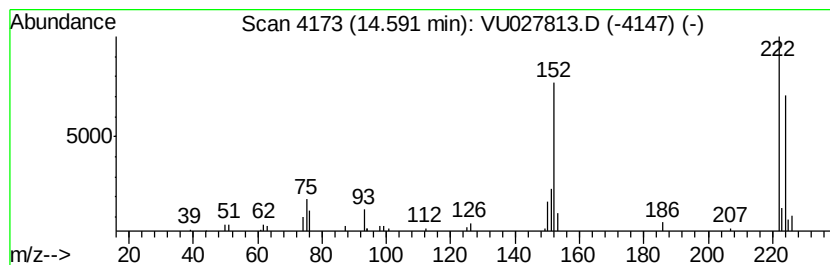
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 1,1'-Biphenyl, 2,3-dichloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.59	11.05 ug/L	69106	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1'-Biphenyl, 2,3-dichloro-	222	C12H8Cl2	016605-91-7	99
2		1,1'-Biphenyl, 2,4'-dichloro-	222	C12H8Cl2	034883-43-7	98
3		1,1'-Biphenyl, 2,5-dichloro-	222	C12H8Cl2	034883-39-1	98
4		1,1'-Biphenyl, 3,4'-dichloro-	222	C12H8Cl2	002974-90-5	98
5		1,1'-Biphenyl 2,3'-dichloro-	222	C12H8Cl2	025569-80-6	98



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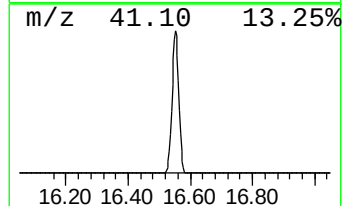
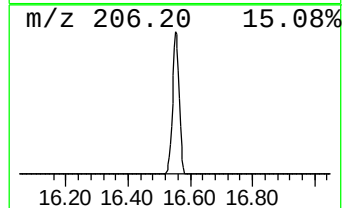
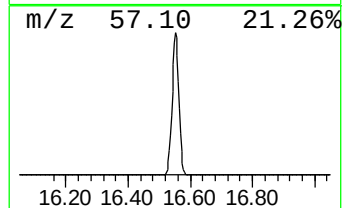
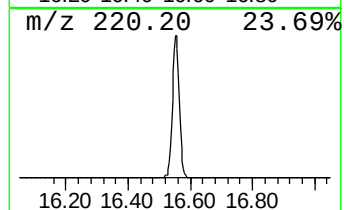
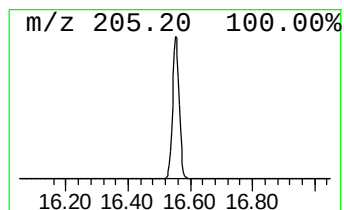
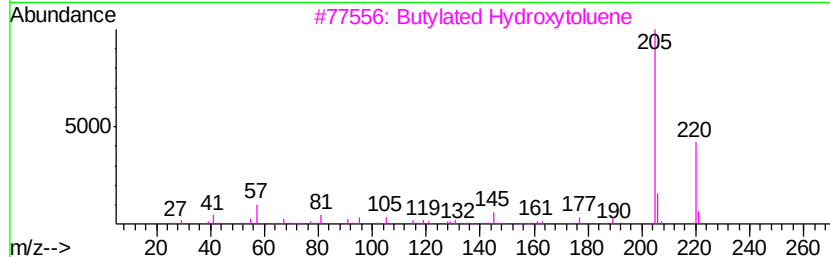
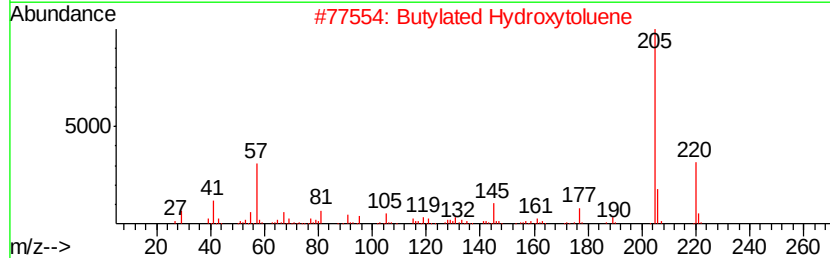
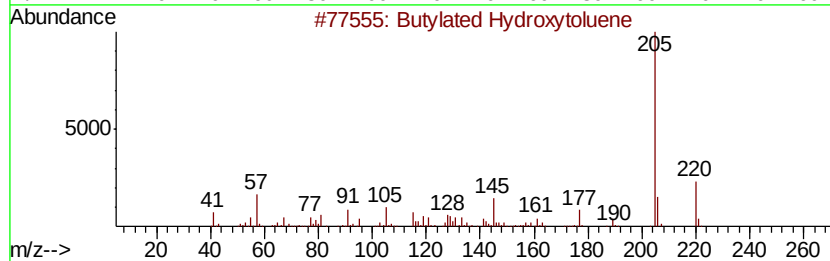
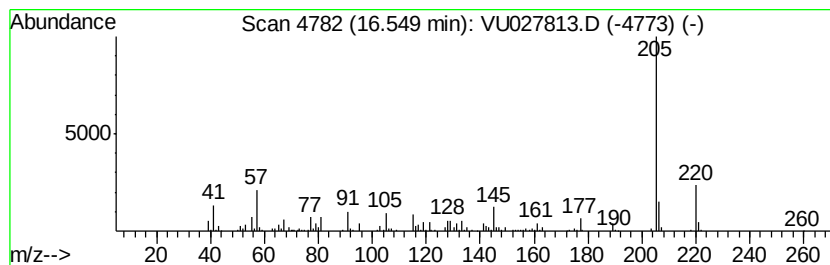
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Quant Title : VOC Analysis

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

Peak Number 5 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.55	27.64 ug/L	172901	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	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1,1'-Biphenyl, 2,...	14.59	11.1	ug/L	69106	3	11.48	312801	50.0
Butylated Hydroxy...	16.55	27.6	ug/L	172901	3	11.48	312801	50.0