

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU102618\
 Data File : VU027824.D
 Acq On : 26 Oct 2018 11:36
 Operator : MD/SY
 Sample : J5635-25ME
 Misc : 4.91g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 8 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	1.395	62	69	85	rVB	34057	42130	9.80%	1.110%
2	1.553	107	118	119	rBV3	4150	4697	1.09%	0.124%
3	1.643	141	146	159	rBV	30379	38480	8.95%	1.013%
4	2.074	278	280	282	rVB	403	177	0.04%	0.005%
5	2.103	282	289	290	rBV3	653	594	0.14%	0.016%
6	2.183	311	314	316	rBV3	322	213	0.05%	0.006%
7	2.238	319	331	345	rVV	61346	95070	22.12%	2.504%
8	2.347	357	365	372	rBV2	444	794	0.18%	0.021%
9	2.443	391	395	399	rBV2	275	283	0.07%	0.007%
10	2.524	417	420	427	rBV2	316	292	0.07%	0.008%
11	2.556	427	430	433	rBV3	255	222	0.05%	0.006%
12	2.624	444	451	456	rBV	363	621	0.14%	0.016%
13	2.833	504	516	533	rVV	5833	12236	2.85%	0.322%
14	2.890	533	534	539	rVV2	316	221	0.05%	0.006%
15	3.485	714	719	724	rBB	213	261	0.06%	0.007%
16	3.717	784	791	797	rBB	191	329	0.08%	0.009%
17	3.781	806	811	817	rBB	156	255	0.06%	0.007%
18	3.816	817	822	825	rBV	183	213	0.05%	0.006%
19	3.919	849	854	857	rBV	130	185	0.04%	0.005%
20	4.099	906	910	916	rBV	193	276	0.06%	0.007%
21	4.196	927	940	991	rBV2	21047	84591	19.68%	2.228%
22	4.485	1025	1030	1031	rBV2	271	200	0.05%	0.005%
23	4.559	1049	1053	1056	rBV	167	181	0.04%	0.005%
24	4.646	1063	1080	1108	rBV	48288	123069	28.63%	3.241%
25	4.784	1117	1123	1126	rBV2	188	251	0.06%	0.007%
26	4.861	1144	1147	1151	rBV	165	194	0.05%	0.005%
27	4.881	1151	1153	1157	rVB2	262	186	0.04%	0.005%
28	4.913	1158	1163	1166	rBV	169	221	0.05%	0.006%
29	4.958	1167	1177	1178	rBV	786	984	0.23%	0.026%
30	5.331	1272	1293	1318	rBV3	108242	319354	74.29%	8.411%
31	5.447	1326	1329	1335	rVB2	478	438	0.10%	0.012%
32	5.517	1348	1351	1354	rBV	179	181	0.04%	0.005%
33	5.652	1389	1393	1396	rBV	170	179	0.04%	0.005%
34	5.884	1451	1465	1493	rBV	119783	249455	58.03%	6.570%

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 ClientSampleId :
 A40G1ME

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
 Title : VOC Analysis

35	6.083	1524	1527	1531	rBB	196	170	0.04%	0.004%
36	6.331	1590	1604	1628	rVB	70259	149923	34.88%	3.949%
37	6.855	1764	1767	1769	rBV2	316	244	0.06%	0.006%
38	6.890	1770	1778	1791	rVV3	1146	2169	0.50%	0.057%
39	7.054	1825	1829	1830	rBV2	305	262	0.06%	0.007%
40	7.067	1831	1833	1838	rVV	345	206	0.05%	0.005%
41	7.231	1871	1884	1907	rVB2	38830	77367	18.00%	2.038%
42	7.492	1962	1965	1968	rVB2	439	339	0.08%	0.009%
43	7.565	1974	1988	2008	rBV	139823	251285	58.45%	6.618%
44	7.633	2008	2009	2013	rVB2	325	175	0.04%	0.005%
45	7.803	2054	2062	2067	rVV2	1154	1819	0.42%	0.048%
46	7.855	2067	2078	2098	rVV2	27100	53614	12.47%	1.412%
47	8.183	2165	2180	2192	rBV2	24063	60198	14.00%	1.585%
48	8.328	2215	2225	2242	rVB	114196	216202	50.29%	5.694%
49	8.498	2274	2278	2281	rBV3	462	393	0.09%	0.010%
50	8.633	2313	2320	2325	rBV5	1624	2501	0.58%	0.066%
51	8.762	2358	2360	2363	rBV2	340	175	0.04%	0.005%
52	8.845	2384	2386	2392	rVB3	939	667	0.16%	0.018%
53	9.093	2451	2463	2480	rBV	188796	331486	77.11%	8.731%
54	10.170	2792	2798	2807	rVB4	2242	3283	0.76%	0.086%
55	10.437	2870	2881	2895	rBV	115602	179048	41.65%	4.716%
56	10.614	2924	2936	2951	rVB2	10642	20627	4.80%	0.543%
57	10.778	2979	2987	2995	rVV3	2936	3877	0.90%	0.102%
58	10.874	3011	3017	3024	rBV2	659	773	0.18%	0.020%
59	11.151	3097	3103	3112	rVV3	2029	2546	0.59%	0.067%
60	11.212	3116	3122	3127	rBV	168	174	0.04%	0.005%
61	11.388	3172	3177	3180	rBV3	805	951	0.22%	0.025%
62	11.421	3180	3187	3196	rVB3	5460	7687	1.79%	0.202%
63	11.485	3196	3207	3231	rVB2	241740	429879	100.00%	11.322%
64	11.572	3231	3234	3238	rVB	361	326	0.08%	0.009%
65	11.630	3249	3252	3256	rVV2	758	692	0.16%	0.018%
66	11.665	3260	3263	3269	rVB4	811	790	0.18%	0.021%
67	11.755	3285	3291	3294	rBV4	1048	1258	0.29%	0.033%
68	11.861	3313	3324	3344	rBV	174645	279705	65.07%	7.367%
69	11.961	3351	3355	3357	rBV	465	316	0.07%	0.008%
70	12.028	3369	3376	3384	rBV4	764	893	0.21%	0.024%
71	12.704	3581	3586	3594	rVB4	2210	3059	0.71%	0.081%

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ClientSampleId :
A40G1ME

Integration Parameters: LSCINT.P

Integrator: RTE
Smoothing : OFF
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72	12.774	3606	3608	3612	rBV2	239	173	0.04%	0.005%
73	12.842	3620	3629	3637	rBV4	1399	2229	0.52%	0.059%
74	12.986	3670	3674	3680	rVB3	201	232	0.05%	0.006%
75	13.128	3710	3718	3723	rBV5	1419	2356	0.55%	0.062%
76	13.749	3906	3911	3915	rBV2	648	740	0.17%	0.019%
77	13.880	3948	3952	3954	rBV	285	211	0.05%	0.006%
78	14.131	4027	4030	4032	rBV	402	190	0.04%	0.005%
79	14.195	4039	4050	4052	rBV2	1180	1763	0.41%	0.046%
80	14.276	4069	4075	4086	rVB	6330	10598	2.47%	0.279%
81	14.327	4089	4091	4093	rBV3	326	180	0.04%	0.005%
82	14.417	4116	4119	4121	rBV	253	196	0.05%	0.005%
83	14.475	4132	4137	4143	rVV4	721	966	0.22%	0.025%
84	14.787	4224	4234	4240	rBV2	15128	21442	4.99%	0.565%
85	14.829	4240	4247	4260	rVV	26889	40176	9.35%	1.058%
86	14.887	4261	4265	4273	rVB3	5145	6210	1.44%	0.164%
87	15.012	4293	4304	4315	rBV2	20957	36409	8.47%	0.959%
88	15.086	4318	4327	4340	rVB2	20795	31742	7.38%	0.836%
89	15.179	4347	4356	4369	rVB2	7112	10024	2.33%	0.264%
90	15.610	4480	4490	4502	rBV	20834	33757	7.85%	0.889%
91	15.880	4565	4574	4585	rBV2	4841	7431	1.73%	0.196%
92	15.935	4589	4591	4596	rBV2	382	242	0.06%	0.006%
93	16.340	4715	4717	4720	rBV	390	228	0.05%	0.006%
94	16.382	4728	4730	4733	rBV3	581	286	0.07%	0.008%
95	16.462	4751	4755	4756	rBV3	730	564	0.13%	0.015%
96	16.552	4771	4783	4796	rVB	269919	399119	92.84%	10.512%
97	16.636	4802	4809	4820	rBV6	2989	4420	1.03%	0.116%
98	16.703	4820	4830	4839	rBV2	29098	45446	10.57%	1.197%
99	17.279	5001	5009	5021	rVB4	12420	18215	4.24%	0.480%
100	17.481	5063	5072	5090	rVB5	31584	59154	13.76%	1.558%

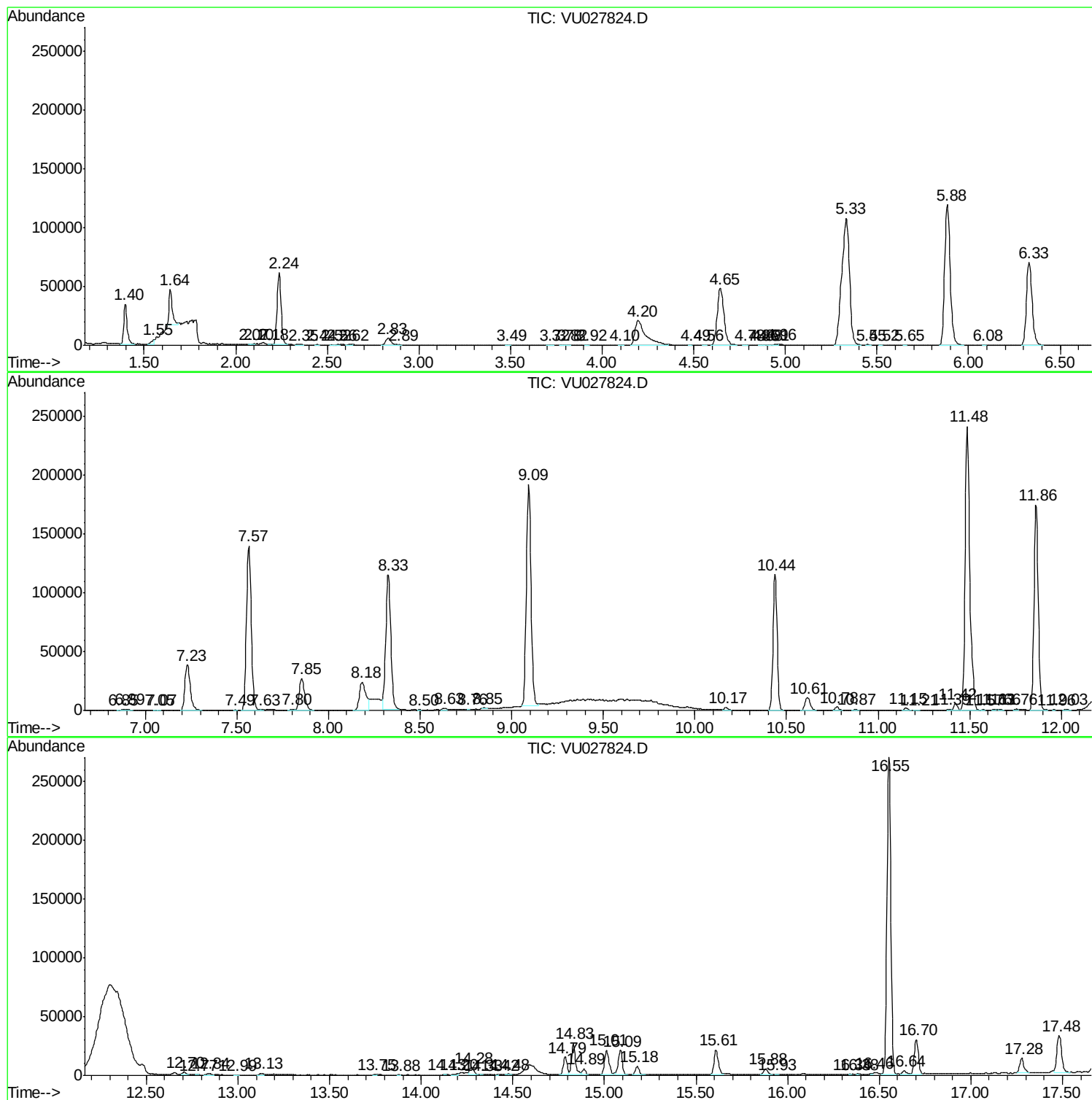
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

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



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Misc : 4.91µ/5mL/100µL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

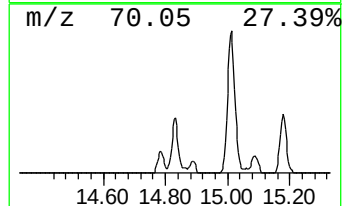
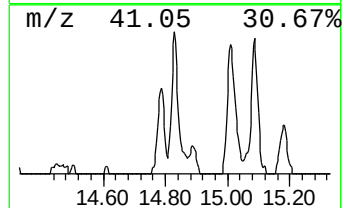
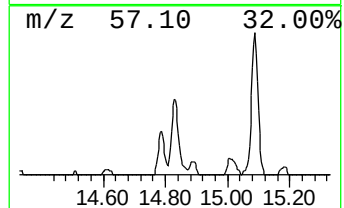
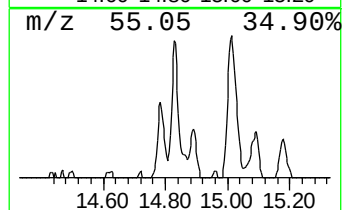
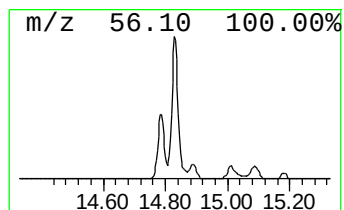
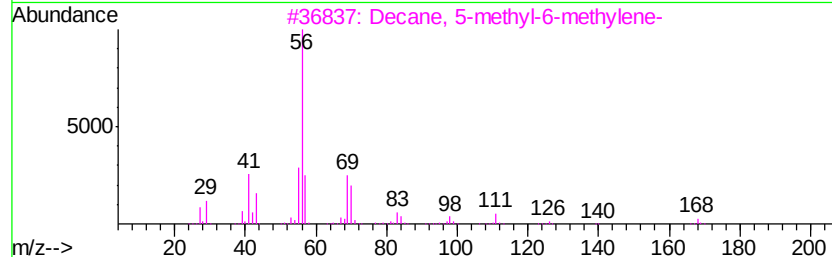
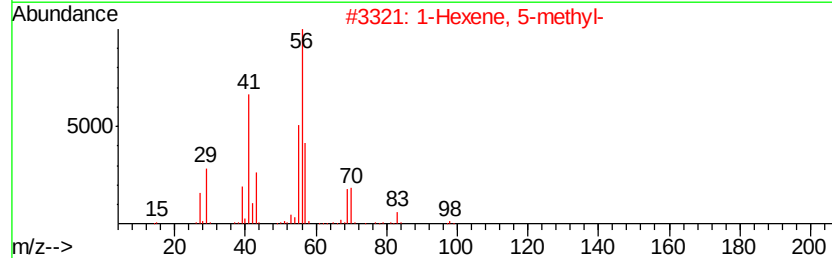
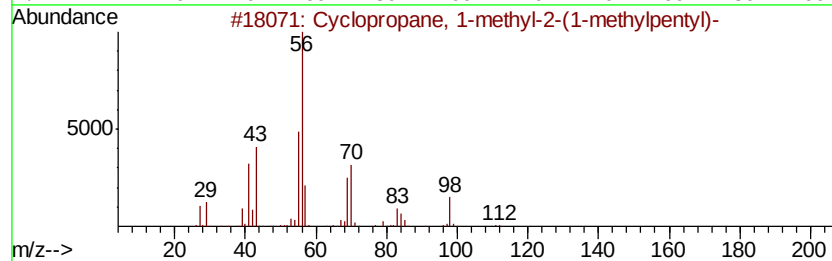
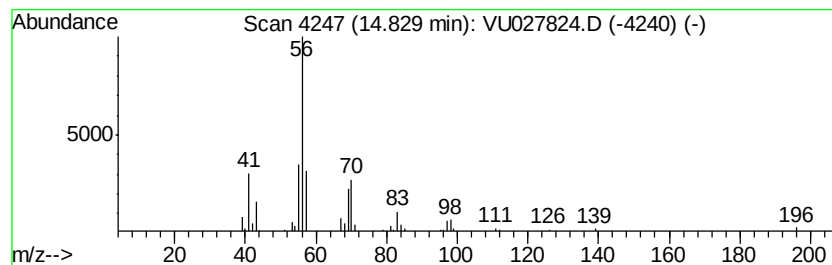
Instrument :
MSVOA_U
ClientSampleId :
A40G1ME

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 3 (DEL) Alkane: Cyclic14.83 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.83	4.67 ug/L	40176	1,4-Dichlorobenzene-d4	11.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1-methyl-2-(1-meth...	140	C10H20	062238-06-6	80
2	1-Hexene, 5-methyl-	98	C7H14	003524-73-0	72
3	Decane, 5-methyl-6-methylene-	168	C12H24	075029-95-7	72
4	1-Decene, 2-methyl-	154	C11H22	013151-27-4	64
5	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	64



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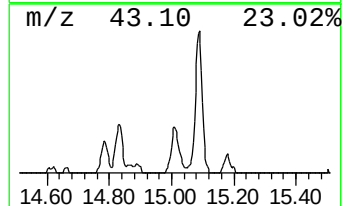
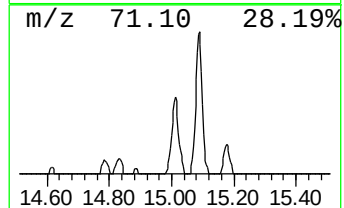
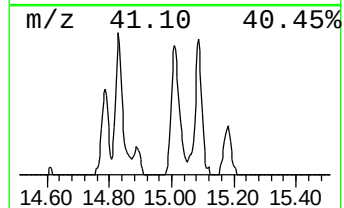
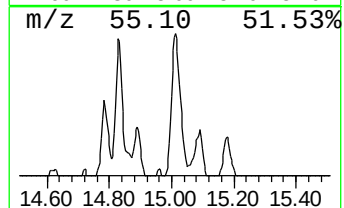
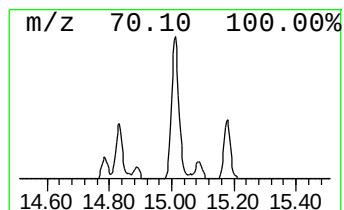
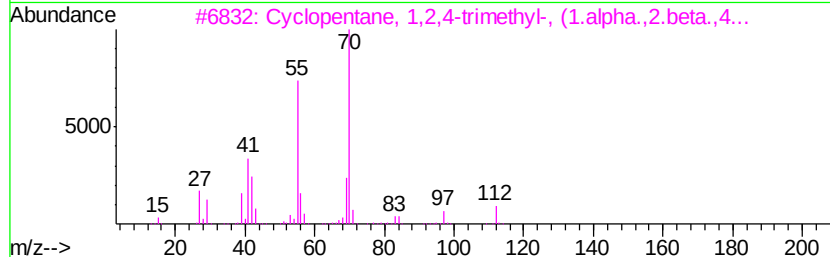
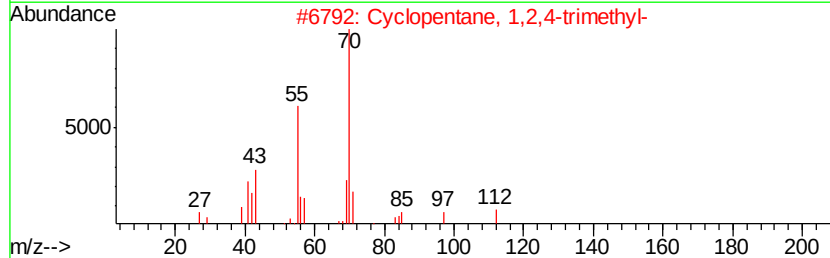
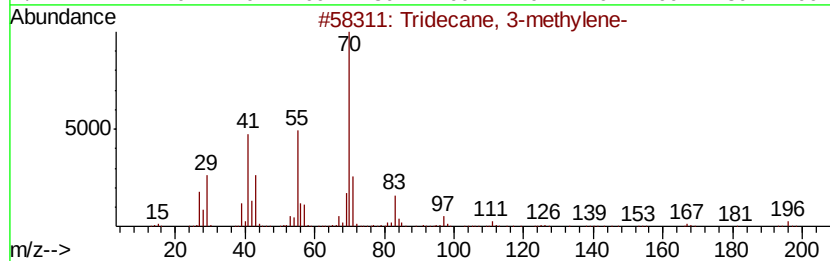
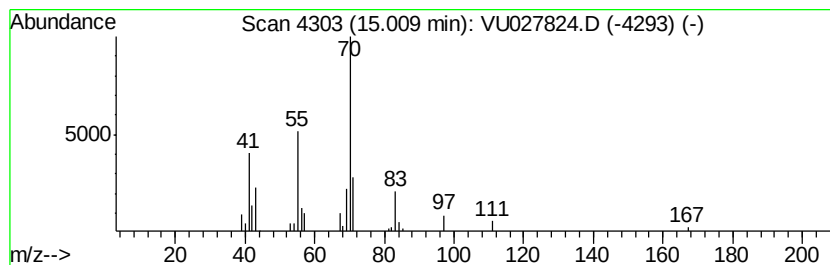
Instrument :
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ClientSampleId :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM102218WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Cyclic15.01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.01	4.23 ug/L	36409	1,4-Dichlorobenzene-d4	11.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane, 3-methylene-	196	C14H28	019780-34-8	80
2	Cyclopentane, 1,2,4-trimethyl-	112	C8H16	002815-58-9	59
3	Cyclopentane, 1,2,4-trimethyl-, ...	112	C8H16	016883-48-0	53
4	Octane, 3-methyl-6-methylene-	140	C10H20	074630-07-2	53
5	Cyclopentane, 1,2,4-trimethyl-	112	C8H16	002815-58-9	53



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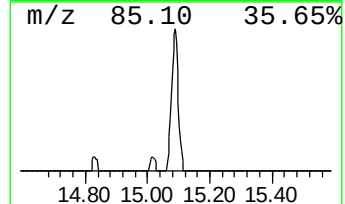
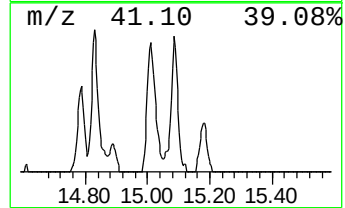
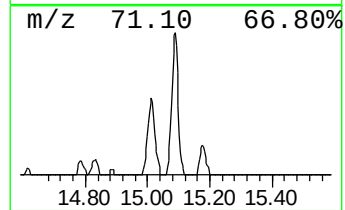
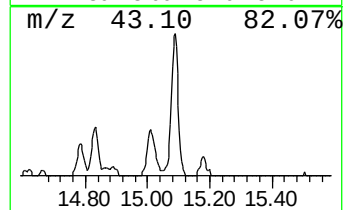
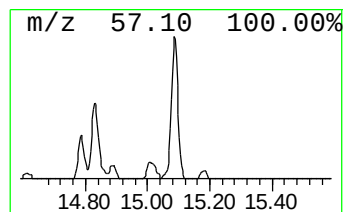
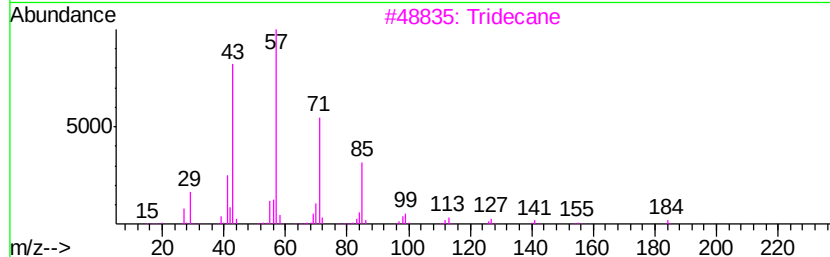
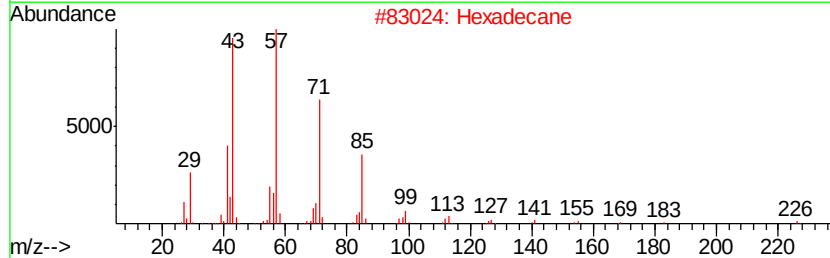
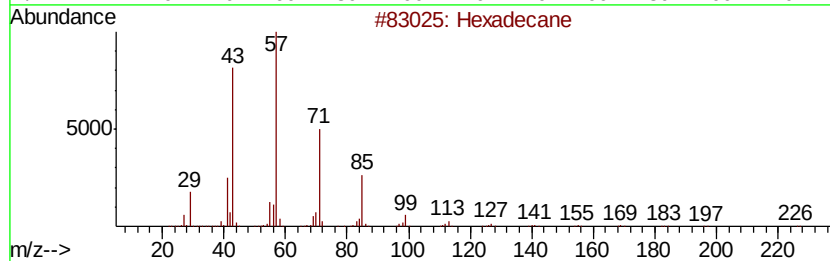
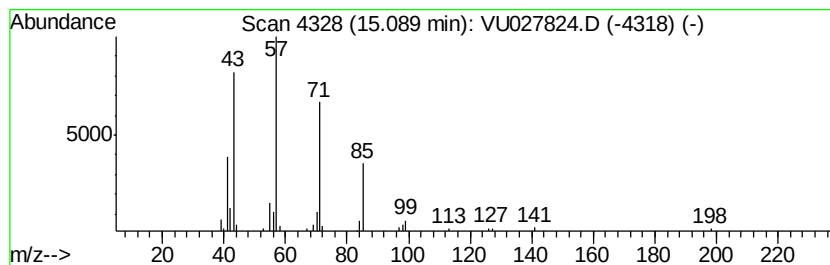
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Quant Title : VOC Analysis

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.09	3.69 ug/L	31742	1,4-Dichlorobenzene-d4	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Hexadecane	226	C16H34	000544-76-3	90
3	Tridecane	184	C13H28	000629-50-5	90
4	Decane, 5-propyl-	184	C13H28	017312-62-8	86
5	Tetradecane	198	C14H30	000629-59-4	83



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU102618\
Data File : VU027824.D
Acq On : 26 Oct 2018 11:36
Operator : MD/SY
Sample : J5635-25ME
Misc : 4.91g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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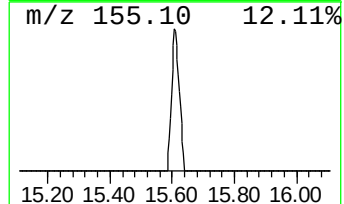
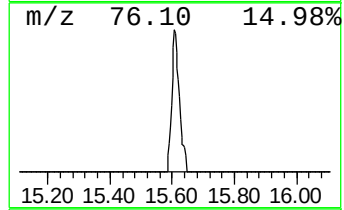
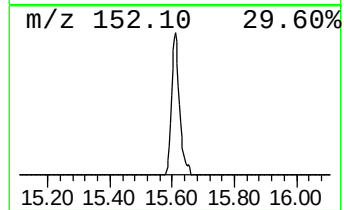
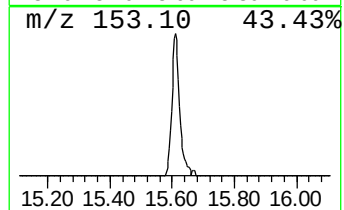
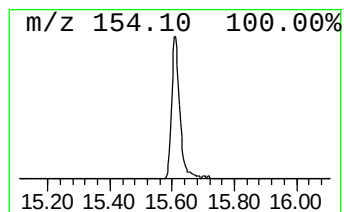
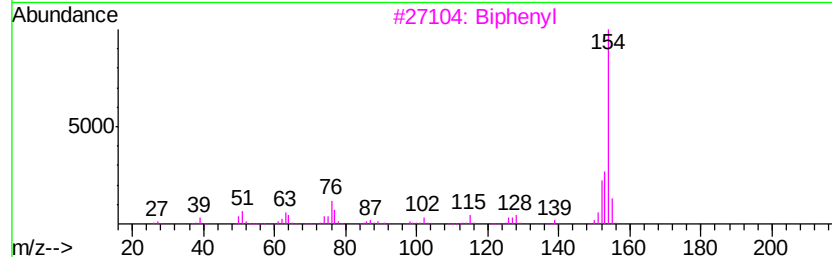
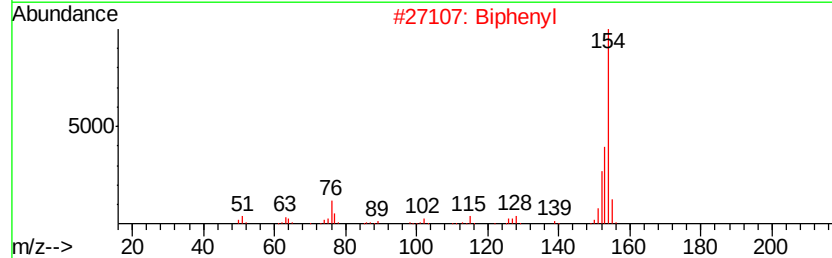
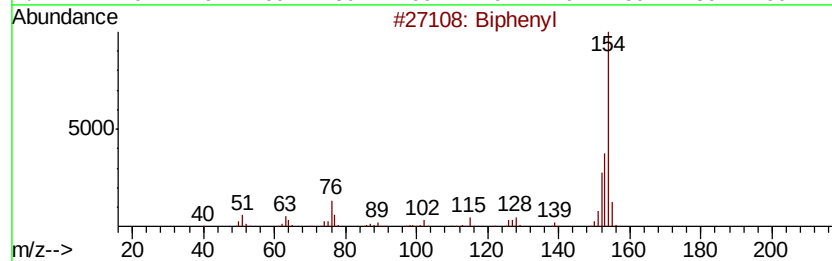
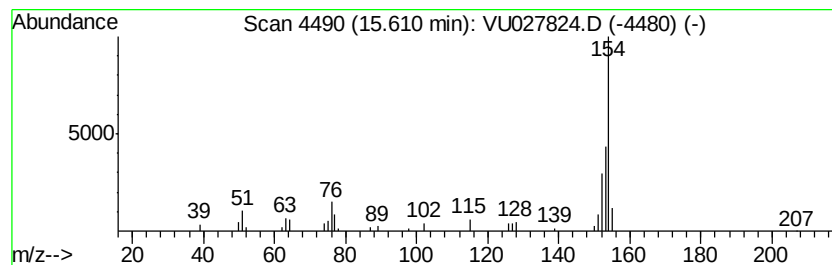
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Quant Title : VOC Analysis

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

Peak Number 6 Biphenyl Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.61	3.93 ug/L	33757	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Biphenyl	154	C12H10	000092-52-4	94
2		Biphenyl	154	C12H10	000092-52-4	94
3		Biphenyl	154	C12H10	000092-52-4	94
4		Biphenyl	154	C12H10	000092-52-4	93
5		Biphenyl	154	C12H10	000092-52-4	93



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU102618\
Data File : VU027824.D
Acq On : 26 Oct 2018 11:36
Operator : MD/SY
Sample : J5635-25ME
Misc : 4.91g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

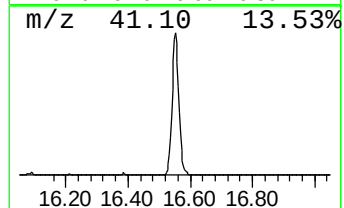
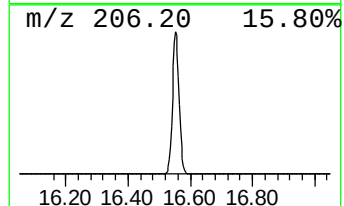
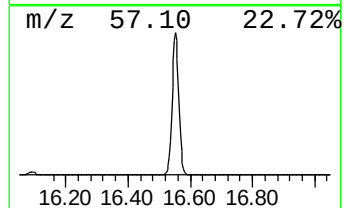
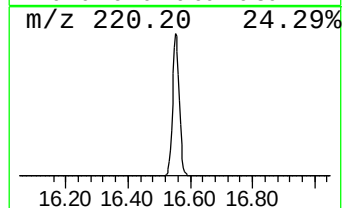
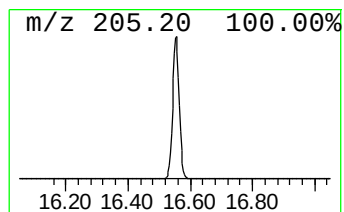
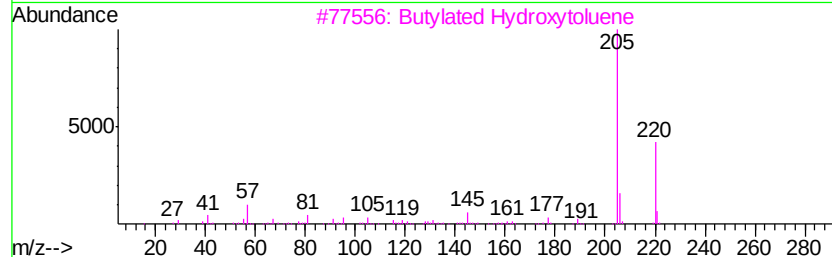
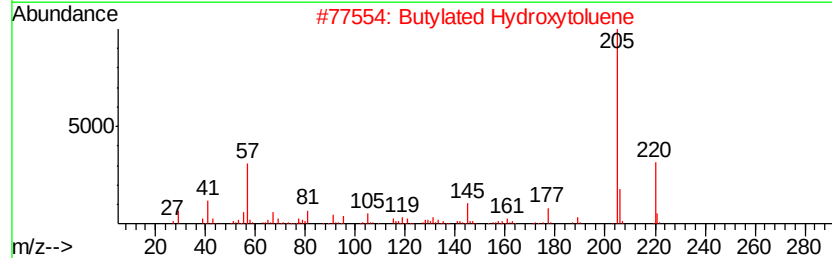
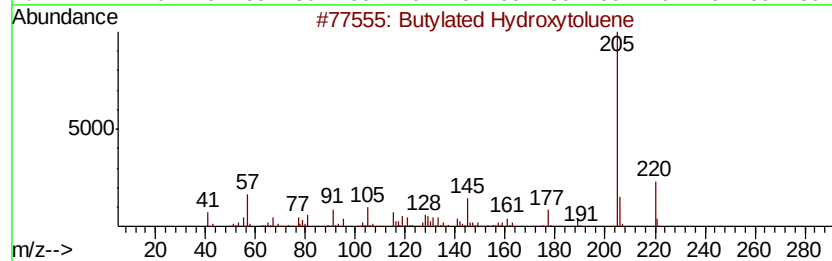
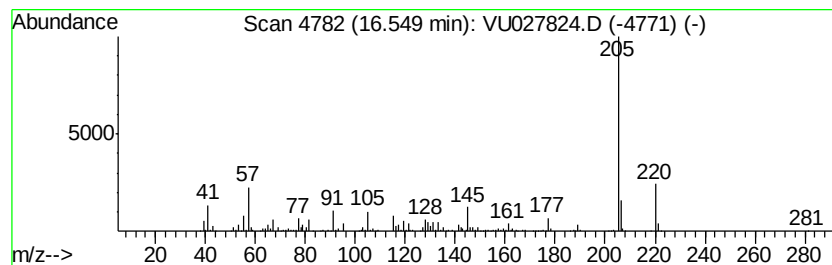
Instrument :
MSVOA_U
ClientSampleId :
A40G1ME

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 7 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.55	46.42 ug/L	399119	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	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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU102618\
Data File : VU027824.D
Acq On : 26 Oct 2018 11:36
Operator : MD/SY
Sample : J5635-25ME
Misc : 4.91g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A40G1ME

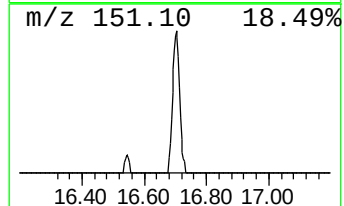
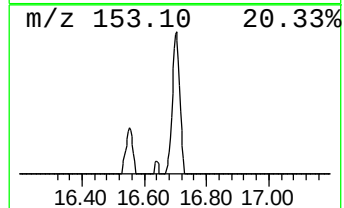
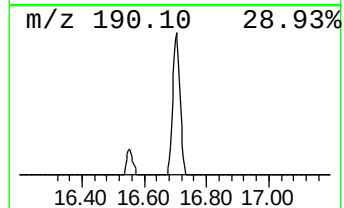
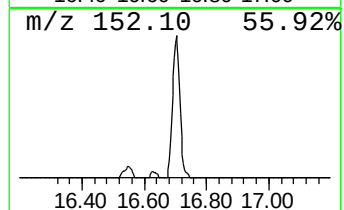
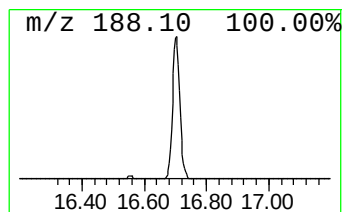
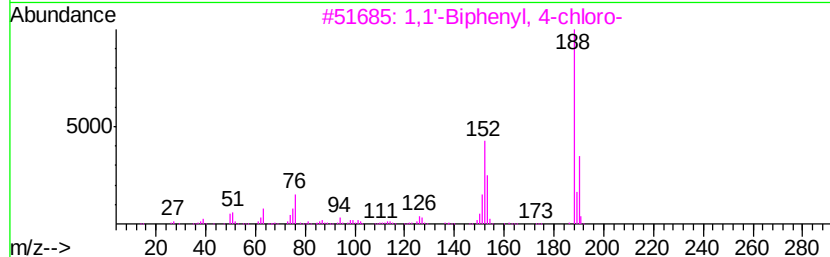
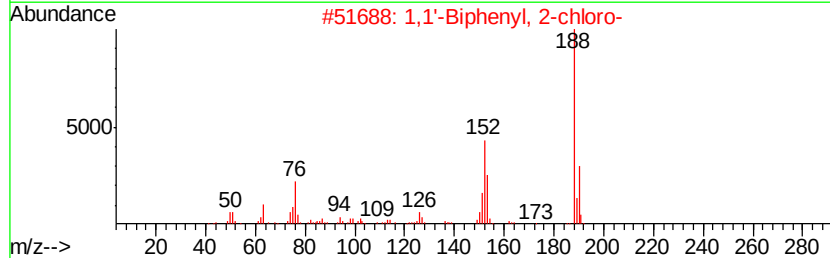
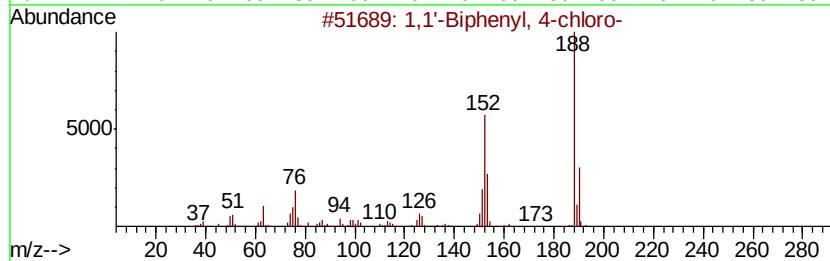
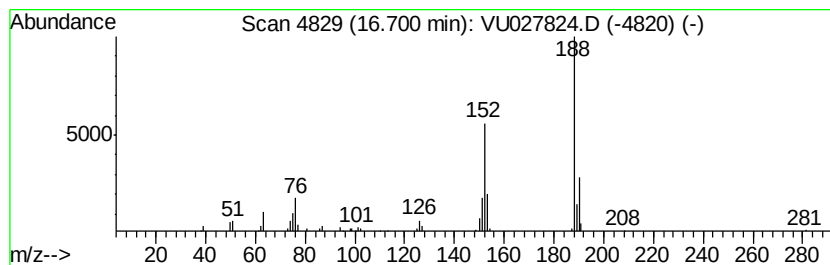
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Quant Title : VOC Analysis

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

Peak Number 8 1,1'-Biphenyl, 4-chloro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.70	5.29 ug/L	45446	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,1'-Biphenyl, 4-chloro-	188	C12H9Cl	002051-62-9	97
2		1,1'-Biphenyl, 2-chloro-	188	C12H9Cl	002051-60-7	96
3		1,1'-Biphenyl, 4-chloro-	188	C12H9Cl	002051-62-9	95
4		3-Chlorobiphenyl	188	C12H9Cl	002051-61-8	94
5		3-Chlorobiphenyl	188	C12H9Cl	002051-61-8	94



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU102618\
Data File : VU027824.D
Acq On : 26 Oct 2018 11:36
Operator : MD/SY
Sample : J5635-25ME
Misc : 4.91g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

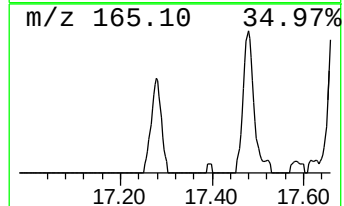
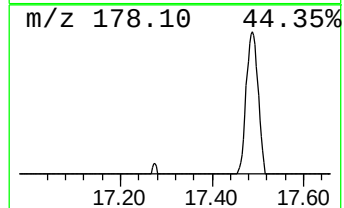
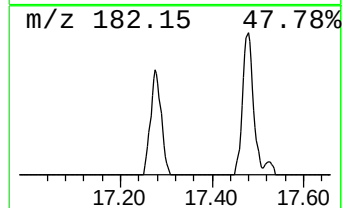
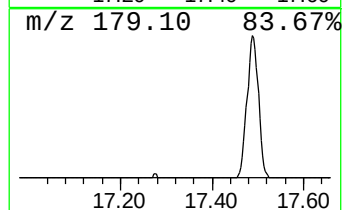
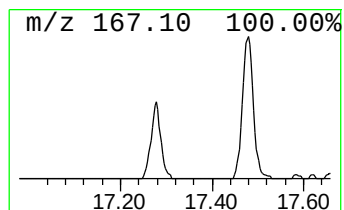
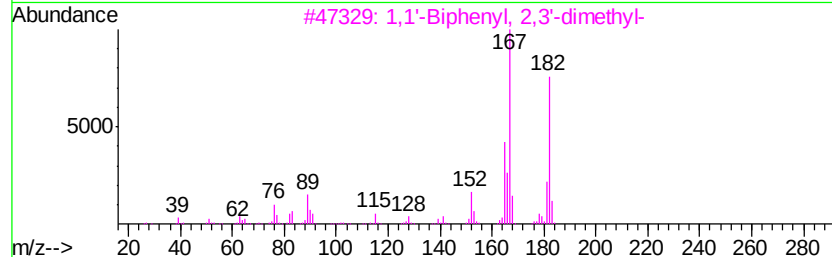
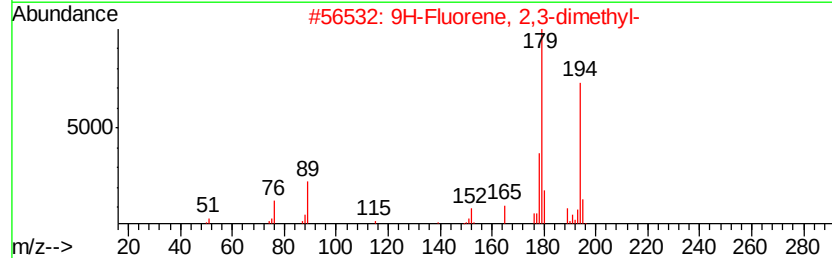
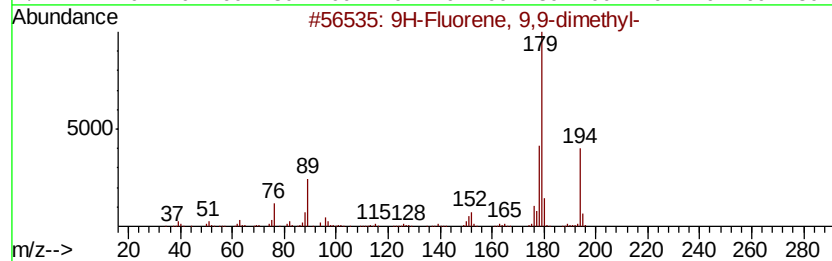
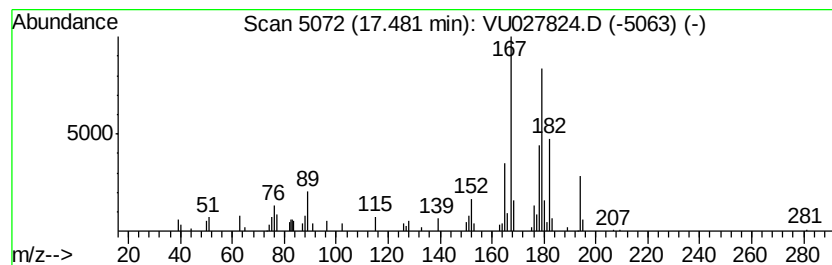
Instrument :
MSVOA_U
ClientSampleId :
A40G1ME

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 9 9H-Fluorene, 9,9-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.48	6.88 ug/L	59154	1,4-Dichlorobenzene-d4	11.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9H-Fluorene, 9,9-dimethyl-	194	C15H14	004569-45-3	89
2	9H-Fluorene, 2,3-dimethyl-	194	C15H14	004612-63-9	50
3	1,1'-Biphenyl, 2,3'-dimethyl-	182	C14H14	000611-43-8	50
4	9H-Fluorene, 9,9-dimethyl-	194	C15H14	004569-45-3	50
5	2,2'-Dimethylbiphenyl	182	C14H14	000605-39-0	46



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU102618\
Data File : VU027824.D
Acq On : 26 Oct 2018 11:36
Operator : MD/SY
Sample : J5635-25ME
Misc : 4.91g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: Cyc...	14.83	4.7	ug/L	40176	3	11.48	429879	50.0
(DEL) Alkane: Cyc...	15.01	4.2	ug/L	36409	3	11.48	429879	50.0
(DEL) Alkane: Str...	15.09	3.7	ug/L	31742	3	11.48	429879	50.0
Biphenyl	15.61	3.9	ug/L	33757	3	11.48	429879	50.0
Butylated Hydroxy...	16.55	46.4	ug/L	399119	3	11.48	429879	50.0
1,1'-Biphenyl, 4-...	16.70	5.3	ug/L	45446	3	11.48	429879	50.0
9H-Fluorene, 9,9-...	17.48	6.9	ug/L	59154	3	11.48	429879	50.0