

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072618\
 Data File : VU025645.D
 Acq On : 26 Jul 2018 11:46
 Operator : MD/SY
 Sample : J4040-08ME
 Misc : 5.14g/5mL/100uL/5.00mL/MSVOA_U/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0AE2ME

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\SOMULM072018WMA.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	0.834	71	76	79	rBV3	301	351	0.02%	0.002%
2	1.011	124	131	138	rBV2	547	752	0.04%	0.005%
3	1.082	138	153	173	rBV	815681	901483	45.01%	6.386%
4	1.394	243	250	270	rBV	91326	139124	6.95%	0.986%
5	1.555	287	300	301	rBV7	10673	15846	0.79%	0.112%
6	1.641	322	327	341	rBV	63081	95269	4.76%	0.675%
7	2.239	502	513	529	rBV	226690	350434	17.50%	2.482%
8	2.516	595	599	605	rBV4	729	938	0.05%	0.007%
9	2.683	646	651	659	rVV7	1344	2073	0.10%	0.015%
10	3.008	748	752	760	rBV3	454	785	0.04%	0.006%
11	4.214	1106	1127	1158	rVB3	165788	539910	26.96%	3.825%
12	4.644	1244	1261	1288	rVB	183657	446084	22.27%	3.160%
13	5.333	1452	1475	1500	rBV2	384775	1106288	55.24%	7.837%
14	5.886	1633	1647	1669	rVB	311889	628022	31.36%	4.449%
15	6.185	1726	1740	1754	rBV	159468	309546	15.46%	2.193%
16	6.329	1772	1785	1803	rBV	243229	497760	24.85%	3.526%
17	7.230	2052	2065	2089	rVB	144269	268338	13.40%	1.901%
18	7.474	2138	2141	2142	rBV2	632	343	0.02%	0.002%
19	7.567	2150	2170	2188	rBV	516983	908388	45.36%	6.435%
20	7.789	2235	2239	2241	rBV2	377	334	0.02%	0.002%
21	7.853	2247	2259	2274	rBV2	101342	184007	9.19%	1.303%
22	8.046	2315	2319	2324	rVB6	940	964	0.05%	0.007%
23	8.120	2339	2342	2351	rBV4	411	572	0.03%	0.004%
24	8.230	2353	2376	2392	rBV	1173192	2002698	100.00%	14.187%
25	8.323	2393	2405	2426	rVB	295326	544730	27.20%	3.859%
26	8.477	2448	2453	2455	rBV5	1433	1429	0.07%	0.010%
27	8.545	2468	2474	2481	rVB5	1921	3014	0.15%	0.021%
28	8.606	2486	2493	2502	rBV4	2350	3539	0.18%	0.025%
29	8.651	2504	2507	2510	rVB3	812	478	0.02%	0.003%
30	8.902	2580	2585	2587	rBV2	516	476	0.02%	0.003%
31	9.094	2632	2645	2661	rBV	466319	787845	39.34%	5.581%
32	9.255	2690	2695	2703	rVB4	1699	1849	0.09%	0.013%
33	9.307	2707	2711	2715	rBV2	403	350	0.02%	0.002%
34	9.377	2721	2733	2747	rBV3	5647	10892	0.54%	0.077%

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Integration Parameters: LSCINT.P

Integrator: RTE
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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
 Title : VOC Analysis

35	9.448	2750	2755	2767	rVB5	1686	2172	0.11%	0.015%
36	9.721	2830	2840	2848	rVB7	1648	3078	0.15%	0.022%
37	9.760	2848	2852	2854	rBV3	512	419	0.02%	0.003%
38	9.783	2854	2859	2861	rBV3	1735	1511	0.08%	0.011%
39	10.008	2921	2929	2932	rBV5	1767	2219	0.11%	0.016%
40	10.088	2947	2954	2962	rVB7	1205	1839	0.09%	0.013%
41	10.152	2962	2974	2990	rVB	151060	251811	12.57%	1.784%
42	10.229	2990	2998	3001	rBV5	952	1227	0.06%	0.009%
43	10.249	3001	3004	3008	rBV4	556	526	0.03%	0.004%
44	10.323	3021	3027	3030	rVV6	1208	1313	0.07%	0.009%
45	10.358	3034	3038	3040	rBV4	755	602	0.03%	0.004%
46	10.438	3051	3063	3077	rBV	408253	653642	32.64%	4.630%
47	10.602	3106	3114	3116	rBV5	1630	1595	0.08%	0.011%
48	10.689	3136	3141	3142	rBV2	1428	1337	0.07%	0.009%
49	10.760	3154	3163	3165	rBV8	2615	2931	0.15%	0.021%
50	10.828	3173	3184	3192	rBV3	30775	53703	2.68%	0.380%
51	10.979	3224	3231	3236	rBV5	1852	2708	0.14%	0.019%
52	11.072	3257	3260	3264	rBV5	1229	934	0.05%	0.007%
53	11.152	3277	3285	3289	rBV6	4775	8097	0.40%	0.057%
54	11.188	3289	3296	3307	rVB2	26505	40520	2.02%	0.287%
55	11.381	3348	3356	3365	rBV8	6219	12579	0.63%	0.089%
56	11.432	3367	3372	3378	rVV6	7953	10236	0.51%	0.073%
57	11.490	3378	3390	3409	rVV	591541	938633	46.87%	6.649%
58	11.570	3409	3415	3424	rVB7	3036	4392	0.22%	0.031%
59	11.667	3442	3445	3456	rVB7	3446	4714	0.24%	0.033%
60	11.776	3471	3479	3486	rBV9	1716	2756	0.14%	0.020%
61	11.866	3494	3507	3522	rBV	646277	1030763	51.47%	7.302%
62	11.975	3538	3541	3543	rBV4	916	618	0.03%	0.004%
63	12.030	3552	3558	3565	rVB7	3360	4417	0.22%	0.031%
64	12.146	3588	3594	3601	rBV6	3566	5382	0.27%	0.038%
65	12.239	3619	3623	3625	rBV4	1293	1038	0.05%	0.007%
66	12.364	3652	3662	3666	rBV8	1920	3268	0.16%	0.023%
67	12.487	3693	3700	3703	rBV7	2184	3202	0.16%	0.023%
68	12.573	3717	3727	3734	rBV5	9933	16120	0.80%	0.114%
69	12.712	3760	3770	3776	rBV5	3161	6030	0.30%	0.043%
70	12.882	3820	3823	3824	rBV2	929	506	0.03%	0.004%
71	12.937	3836	3840	3842	rBV3	444	366	0.02%	0.003%

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72	12.966	3845	3849	3855	rVV4	2243	2506	0.13%	0.018%
73	13.056	3874	3877	3880	rVB2	1037	715	0.04%	0.005%
74	13.091	3885	3888	3891	rBV4	924	821	0.04%	0.006%
75	13.126	3892	3899	3910	rVB6	10125	15524	0.78%	0.110%
76	13.191	3916	3919	3926	rVB5	1251	1221	0.06%	0.009%
77	13.220	3926	3928	3930	rBV2	662	376	0.02%	0.003%
78	13.287	3946	3949	3960	rVB9	2441	3424	0.17%	0.024%
79	13.461	3995	4003	4010	rVB7	2005	3136	0.16%	0.022%
80	13.509	4010	4018	4025	rBV9	3835	6040	0.30%	0.043%
81	13.747	4081	4092	4117	rVB	93149	156079	7.79%	1.106%
82	13.840	4117	4121	4123	rBV4	1007	791	0.04%	0.006%
83	13.934	4146	4150	4152	rBV3	1024	870	0.04%	0.006%
84	14.155	4210	4219	4228	rBV8	3838	7518	0.38%	0.053%
85	14.310	4265	4267	4268	rBV2	798	360	0.02%	0.003%
86	14.339	4269	4276	4286	rVB7	4895	9564	0.48%	0.068%
87	14.721	4393	4395	4399	rBV5	942	688	0.03%	0.005%
88	14.747	4399	4403	4406	rBV5	1531	1184	0.06%	0.008%
89	14.882	4433	4445	4456	rBV	88841	147906	7.39%	1.048%
90	15.065	4491	4502	4517	rBV	157713	259945	12.98%	1.841%
91	15.294	4568	4573	4575	rBV5	4360	4706	0.23%	0.033%
92	15.612	4666	4672	4680	rVB2	16513	26245	1.31%	0.186%
93	15.805	4725	4732	4739	rBV	25432	37814	1.89%	0.268%
94	15.917	4757	4767	4777	rBV	72091	128985	6.44%	0.914%
95	16.065	4803	4813	4819	rBV	143013	225780	11.27%	1.599%
96	16.265	4867	4875	4877	rBV	31368	39970	2.00%	0.283%
97	16.435	4922	4928	4938	rVB3	27054	40720	2.03%	0.288%
98	16.548	4954	4963	4977	rBV6	19887	43706	2.18%	0.310%
99	16.740	5016	5023	5031	rBV2	60881	90570	4.52%	0.642%
100	16.917	5074	5078	5090	rBV3	16170	27309	1.36%	0.193%

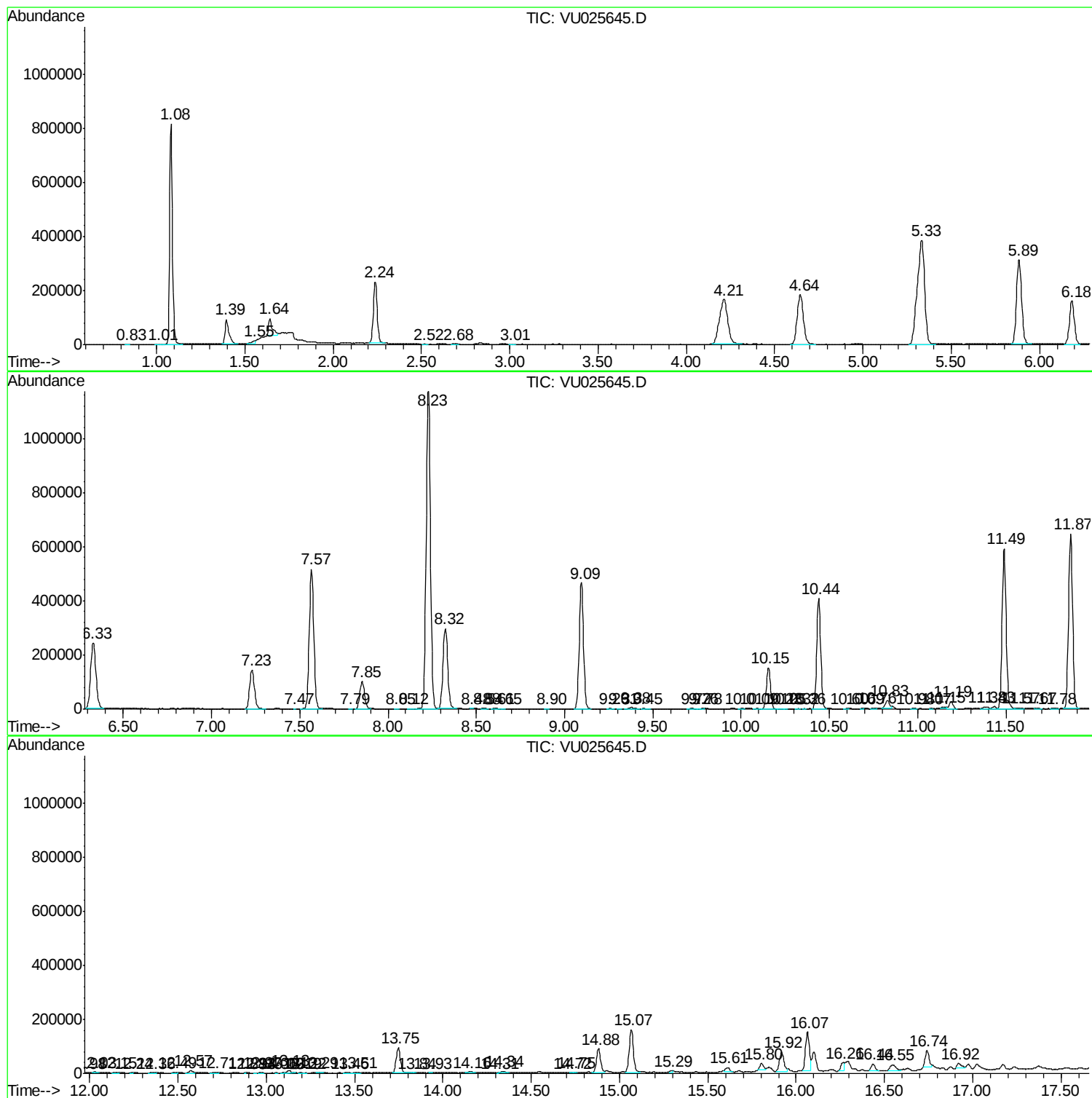
Sum of corrected areas: 14116588

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Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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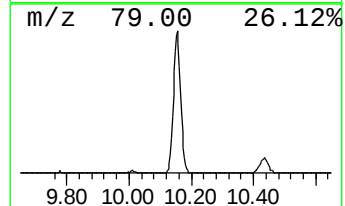
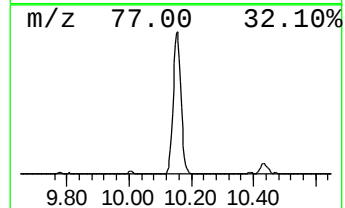
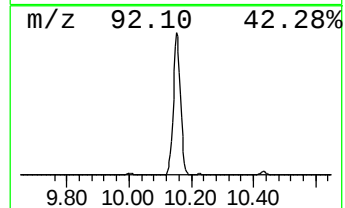
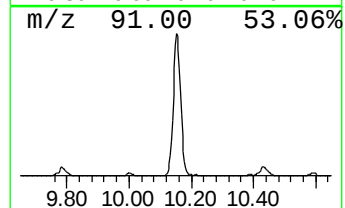
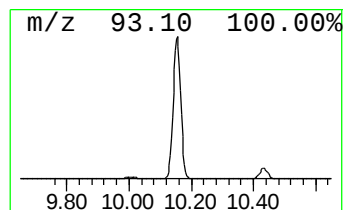
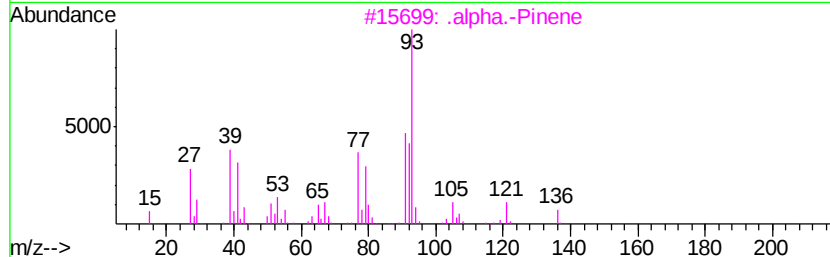
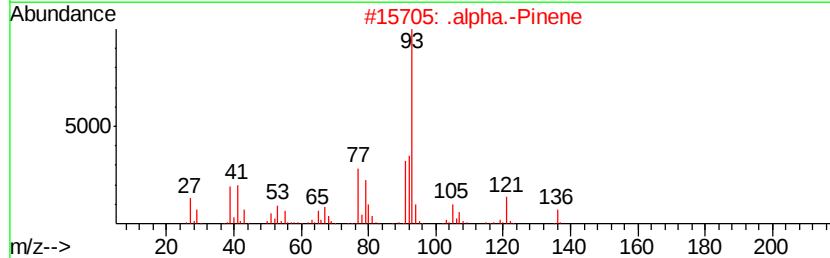
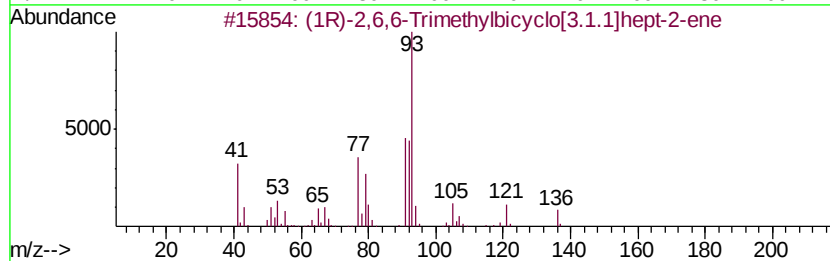
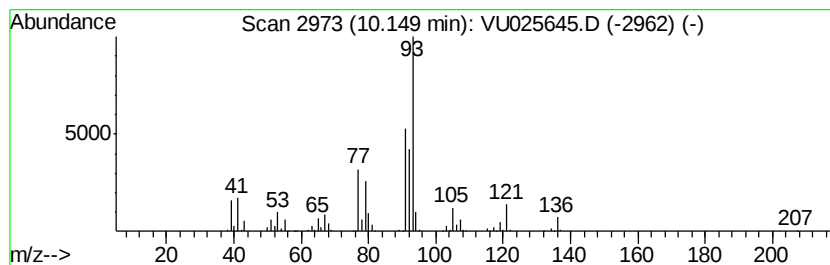
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (1R)-2,6,6-Trimethylbicyclo... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.15	15.98 ug/L	251811	Chlorobenzene-d5	9.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	96
2		.alpha.-Pinene	136	C10H16	000080-56-8	95
3		.alpha.-Pinene	136	C10H16	000080-56-8	95
4		.alpha.-Pinene	136	C10H16	000080-56-8	91
5		(1S)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-26-4	90



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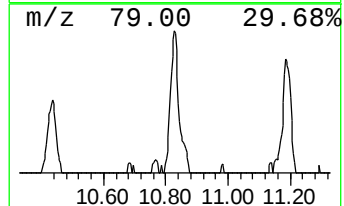
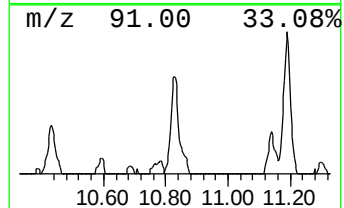
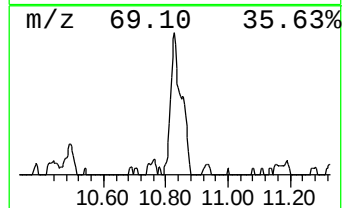
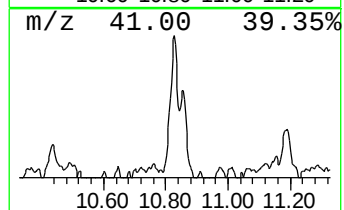
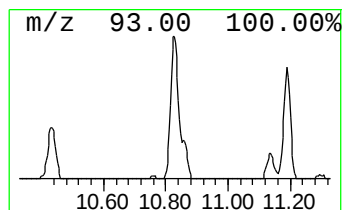
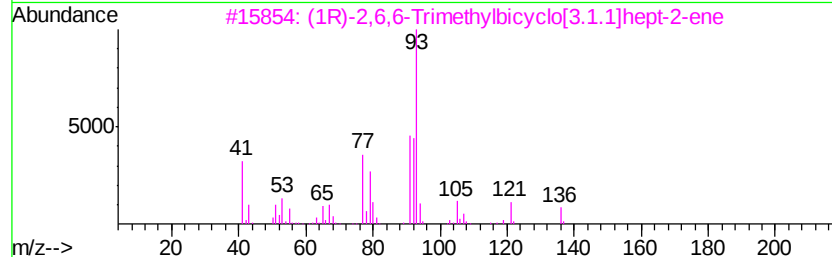
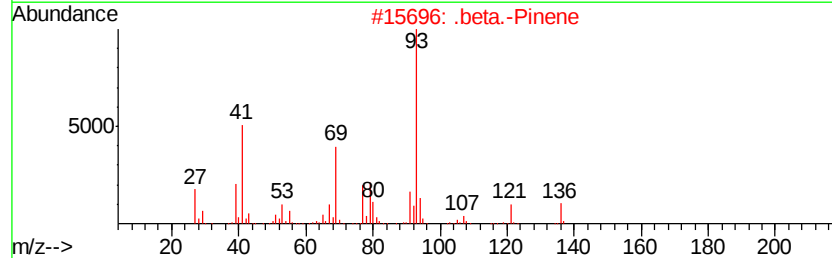
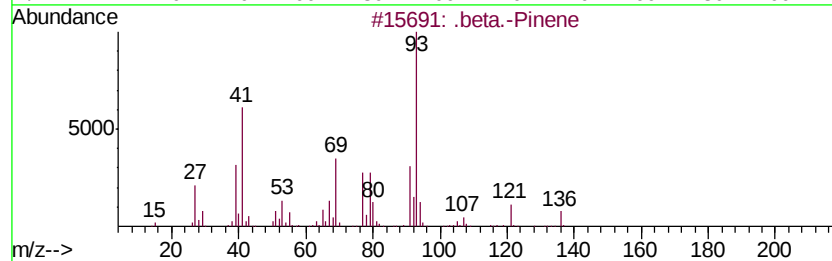
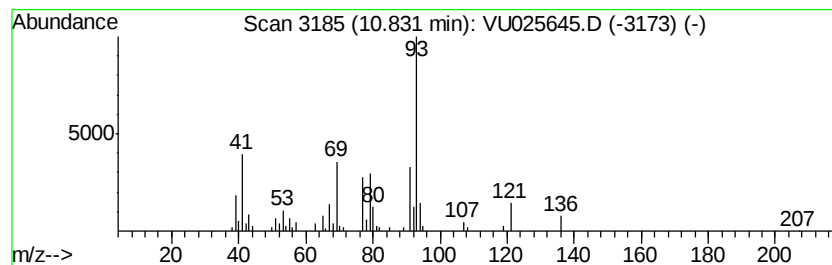
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Quant Title : VOC Analysis

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

Peak Number 4 .beta.-Pinene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.83	2.86 ug/L	53703	1,4-Dichlorobenzene-d4	11.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		.beta.-Pinene	136 C10H16	000127-91-3 97
2		.beta.-Pinene	136 C10H16	000127-91-3 91
3		(1R)-2,6,6-Trimethylbicyclo[3.1....	136 C10H16	007785-70-8 91
4		Cyclohexene, 4-methylene-1-(1-me...	136 C10H16	000099-84-3 91
5		Bicyclo[3.1.0]hexane, 4-methylen...	136 C10H16	003387-41-5 87



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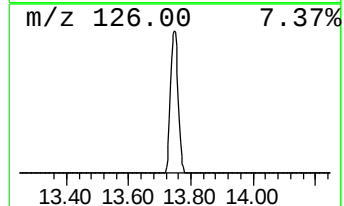
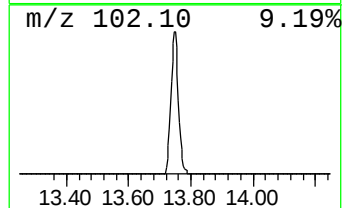
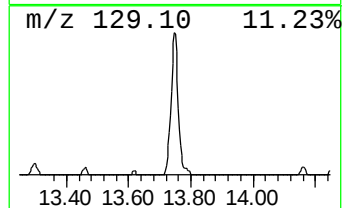
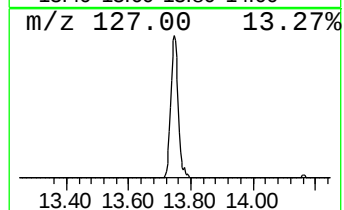
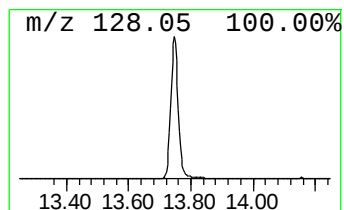
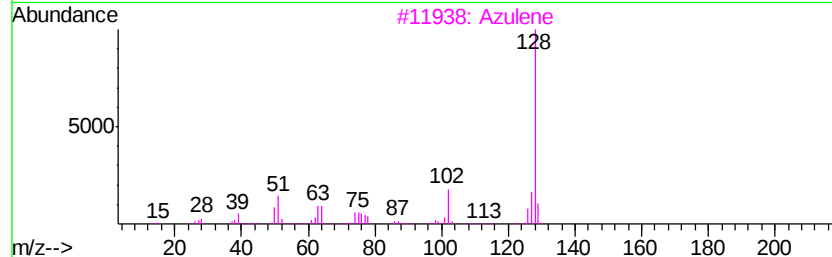
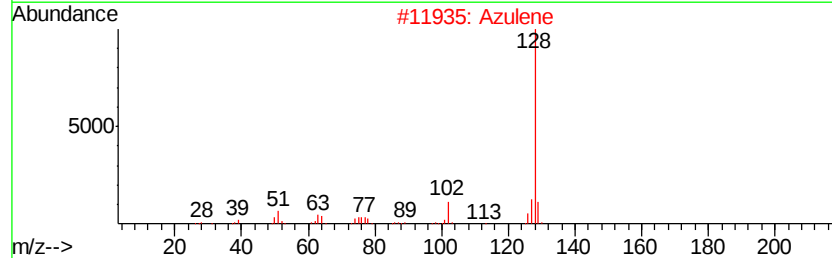
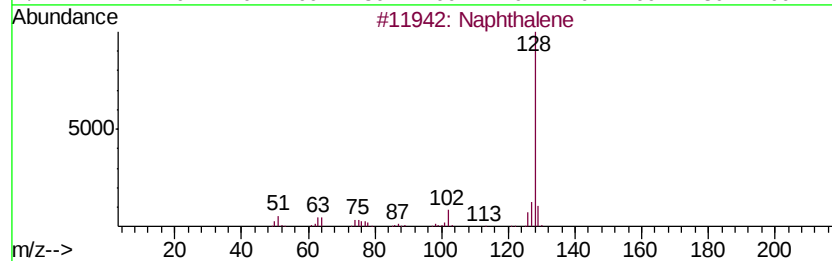
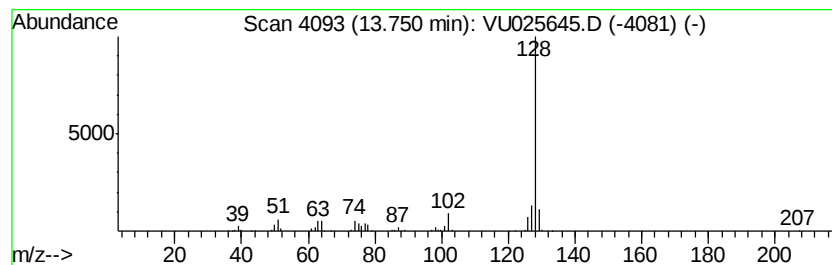
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Quant Title : VOC Analysis

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

Peak Number 5 Azulene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.75	8.31 ug/L	156079	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene	128	C10H8	000091-20-3	95
2		Azulene	128	C10H8	000275-51-4	94
3		Azulene	128	C10H8	000275-51-4	91
4		Naphthalene	128	C10H8	000091-20-3	91
5		Naphthalene	128	C10H8	000091-20-3	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072618\
Data File : VU025645.D
Acq On : 26 Jul 2018 11:46
Operator : MD/SY
Sample : J4040-08ME
Misc : 5.14g/5mL/100uL/5.00mL/MSVOA_U/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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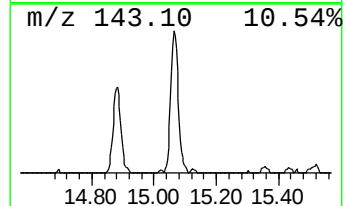
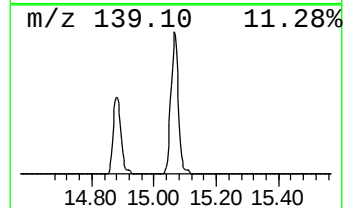
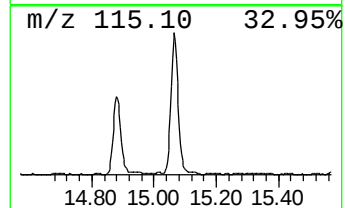
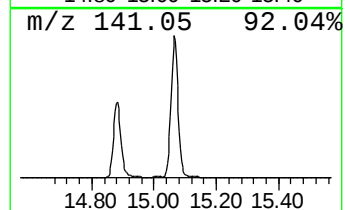
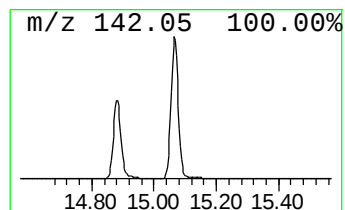
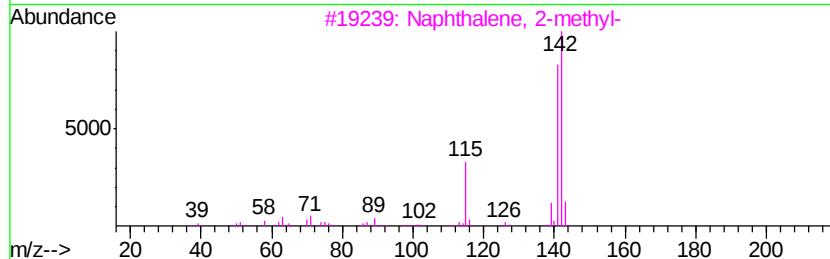
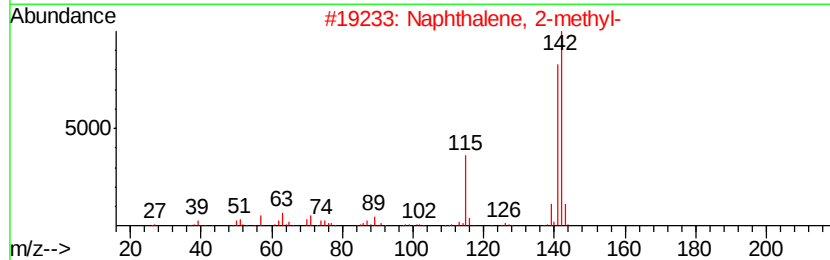
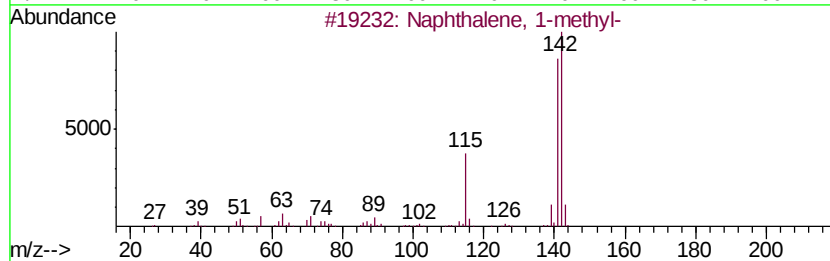
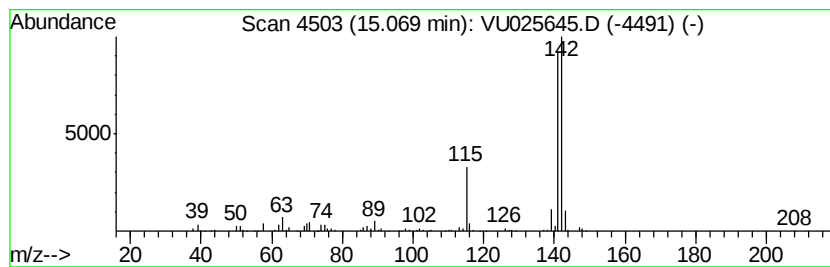
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Quant Title : VOC Analysis

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

Peak Number 7 Naphthalene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.07	13.85 ug/L	259945	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
4		1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	94
5		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072618\
Data File : VU025645.D
Acq On : 26 Jul 2018 11:46
Operator : MD/SY
Sample : J4040-08ME
Misc : 5.14g/5mL/100uL/5.00mL/MSVOA_U/MEOH
ALS Vial : 5 Sample Multiplier: 1

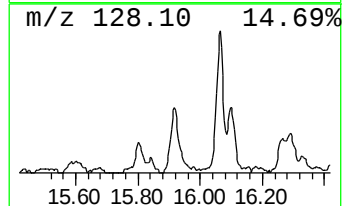
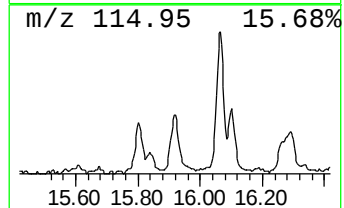
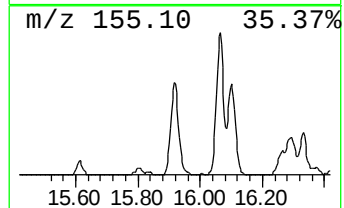
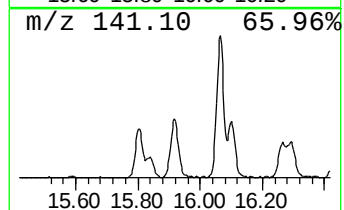
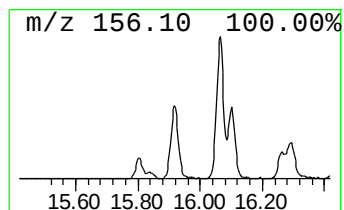
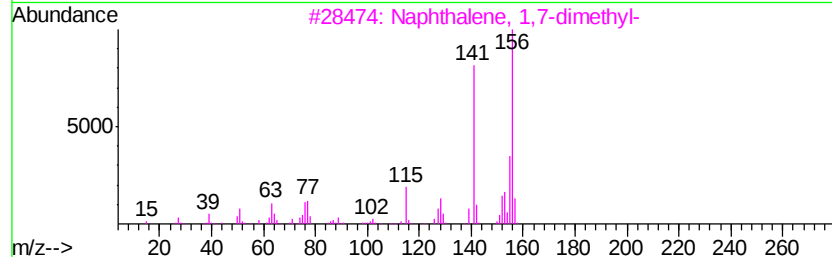
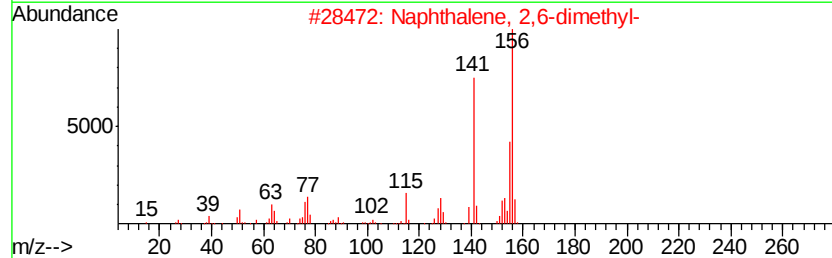
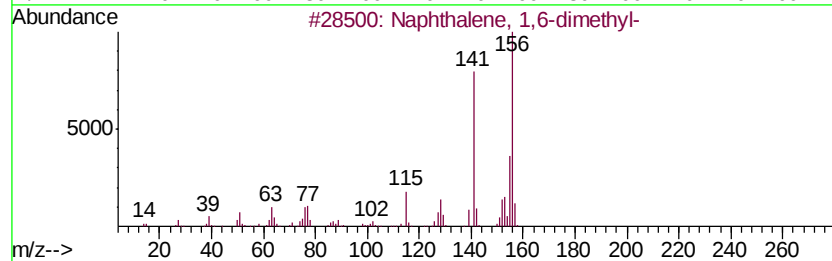
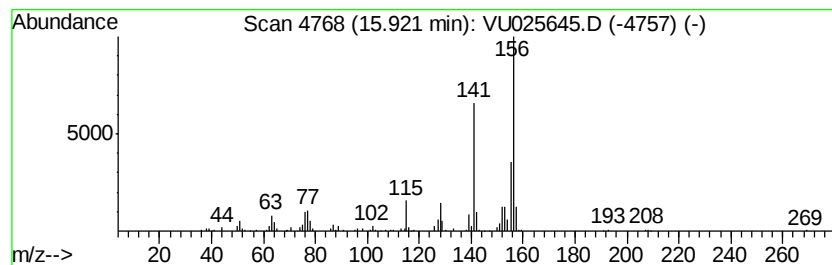
Instrument :
MSVOA_U
ClientSampleId :
C0AE2ME

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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

Peak Number 8 Naphthalene, 1,6-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.92	6.87 ug/L	128985	1,4-Dichlorobenzene-d4	11.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Naphthalene, 1,6-dimethyl-	156 C12H12	000575-43-9 98
2		Naphthalene, 2,6-dimethyl-	156 C12H12	000581-42-0 98
3		Naphthalene, 1,7-dimethyl-	156 C12H12	000575-37-1 98
4		Naphthalene, 2,6-dimethyl-	156 C12H12	000581-42-0 97
5		Naphthalene, 2,7-dimethyl-	156 C12H12	000582-16-1 97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072618\
Data File : VU025645.D
Acq On : 26 Jul 2018 11:46
Operator : MD/SY
Sample : J4040-08ME
Misc : 5.14g/5mL/100uL/5.00mL/MSVOA_U/MEOH
ALS Vial : 5 Sample Multiplier: 1

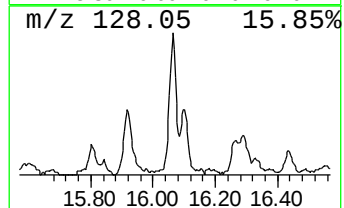
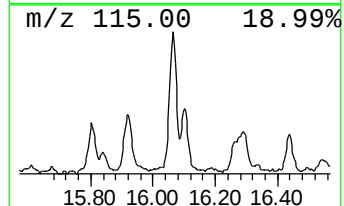
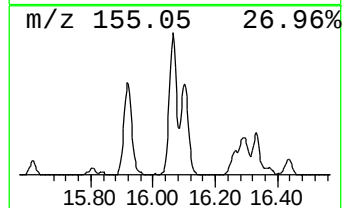
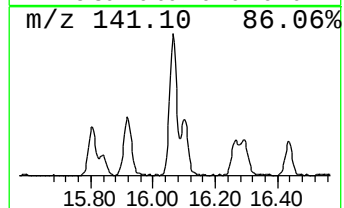
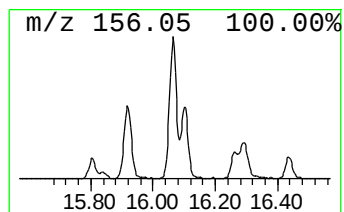
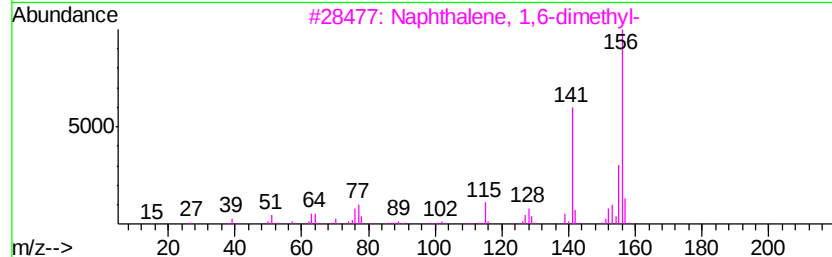
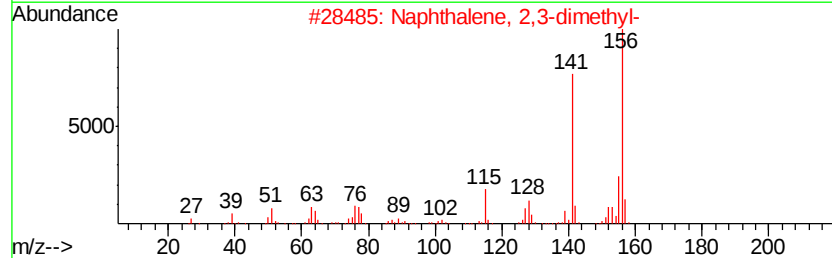
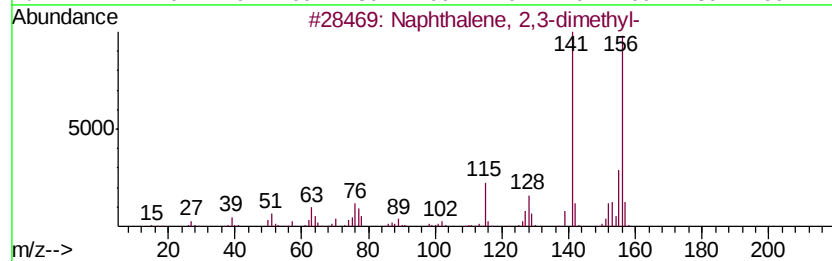
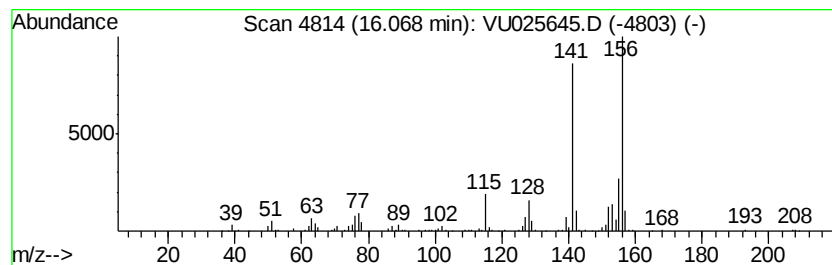
Instrument :
MSVOA_U
ClientSampleId :
C0AE2ME

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.M
Quant Title : VOC Analysis

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

Peak Number 9 Naphthalene, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	12.03 ug/L	225780	1,4-Dichlorobenzene-d4	11.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Naphthalene, 2,3-dimethyl-	156 C12H12	000581-40-8 98
2		Naphthalene, 2,3-dimethyl-	156 C12H12	000581-40-8 97
3		Naphthalene, 1,6-dimethyl-	156 C12H12	000575-43-9 97
4		Naphthalene, 1,4-dimethyl-	156 C12H12	000571-58-4 97
5		Naphthalene, 1,3-dimethyl-	156 C12H12	000575-41-7 96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072618\
Data File : VU025645.D
Acq On : 26 Jul 2018 11:46
Operator : MD/SY
Sample : J4040-08ME
Misc : 5.14g/5mL/100uL/5.00mL/MSVOA_U/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AE2ME

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM072018WMA.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
(1R)-2,6,6-Trimet...	10.15	16.0	ug/L	251811	2	9.09	787845	50.0
.beta.-Pinene	10.83	2.9	ug/L	53703	3	11.49	938633	50.0
Azulene	13.75	8.3	ug/L	156079	3	11.49	938633	50.0
Naphthalene, 1-me...	15.07	13.9	ug/L	259945	3	11.49	938633	50.0
Naphthalene, 1,6-...	15.92	6.9	ug/L	128985	3	11.49	938633	50.0
Naphthalene, 2,3-...	16.07	12.0	ug/L	225780	3	11.49	938633	50.0