

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\U102918\
 Data File : VU027848.D
 Acq On : 29 Oct 2018 11:47
 Operator : MD/SY
 Sample : J5635-25ME
 Misc : 4.91g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 5 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	86	rVB	72773	90447	13.37%	1.428%
2	1.559	108	120	121	rBV4	5101	7263	1.07%	0.115%
3	1.643	140	146	158	rBV	67834	89003	13.15%	1.405%
4	1.826	197	203	213	rVB5	2060	3313	0.49%	0.052%
5	2.087	282	284	287	rBV2	465	351	0.05%	0.006%
6	2.238	320	331	348	rBV	133666	207788	30.71%	3.280%
7	2.440	390	394	398	rBV2	396	450	0.07%	0.007%
8	2.572	429	435	441	rBV2	267	354	0.05%	0.006%
9	2.611	443	447	448	rVV	280	200	0.03%	0.003%
10	2.627	448	452	463	rVB2	669	852	0.13%	0.013%
11	2.707	474	477	483	rVB	233	173	0.03%	0.003%
12	2.833	506	516	531	rBV2	1907	4318	0.64%	0.068%
13	3.723	789	793	797	rBV	164	226	0.03%	0.004%
14	4.196	925	940	990	rBV	42614	163364	24.14%	2.578%
15	4.646	1062	1080	1109	rVV	101925	259713	38.38%	4.099%
16	4.781	1116	1122	1128	rBV2	228	363	0.05%	0.006%
17	4.961	1167	1178	1180	rBV2	752	1194	0.18%	0.019%
18	5.199	1249	1252	1258	rBV	196	264	0.04%	0.004%
19	5.334	1271	1294	1320	rBV2	232514	676649	100.00%	10.680%
20	5.485	1338	1341	1344	rBV2	244	206	0.03%	0.003%
21	5.685	1398	1403	1406	rBV	182	237	0.04%	0.004%
22	5.775	1425	1431	1433	rBV	160	222	0.03%	0.004%
23	5.884	1451	1465	1493	rBV	154405	324166	47.91%	5.116%
24	6.170	1548	1554	1555	rBV2	574	478	0.07%	0.008%
25	6.331	1589	1604	1631	rBV	146571	316966	46.84%	5.003%
26	6.463	1642	1645	1649	rVV	225	171	0.03%	0.003%
27	6.543	1663	1670	1675	rBV	199	395	0.06%	0.006%
28	6.865	1762	1770	1772	rBV2	998	1222	0.18%	0.019%
29	7.054	1823	1829	1833	rBV2	364	522	0.08%	0.008%
30	7.228	1870	1883	1905	rBV	85653	169960	25.12%	2.683%
31	7.382	1926	1931	1933	rBV2	730	670	0.10%	0.011%
32	7.395	1933	1935	1941	rVB4	519	497	0.07%	0.008%
33	7.566	1974	1988	2007	rBV	307672	550713	81.39%	8.692%
34	7.807	2053	2063	2067	rBV4	1402	2148	0.32%	0.034%

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 Title : VOC Analysis

35	7.852	2067	2077	2100	rVB	59596	116907	17.28%	1.845%
36	8.183	2167	2180	2189	rBV2	14475	34919	5.16%	0.551%
37	8.324	2213	2224	2259	rVB	239161	432637	63.94%	6.828%
38	8.521	2283	2285	2292	rVB2	359	250	0.04%	0.004%
39	8.633	2313	2320	2328	rVB2	1192	1923	0.28%	0.030%
40	8.678	2329	2334	2336	rBV	199	232	0.03%	0.004%
41	8.849	2383	2387	2395	rVB2	692	817	0.12%	0.013%
42	9.048	2445	2449	2451	rBV2	445	402	0.06%	0.006%
43	9.093	2451	2463	2483	rVV	240872	416092	61.49%	6.567%
44	9.382	2547	2553	2555	rBV	308	297	0.04%	0.005%
45	9.566	2607	2610	2616	rBV	147	162	0.02%	0.003%
46	9.787	2675	2679	2685	rVB3	536	585	0.09%	0.009%
47	9.958	2726	2732	2742	rVB3	977	1299	0.19%	0.021%
48	10.170	2788	2798	2808	rBV2	2509	3389	0.50%	0.053%
49	10.437	2869	2881	2902	rVV	234730	367424	54.30%	5.799%
50	10.617	2925	2937	2951	rVB2	6924	13561	2.00%	0.214%
51	10.774	2979	2986	2995	rVV2	2857	3898	0.58%	0.062%
52	10.813	2996	2998	3002	rVB2	386	203	0.03%	0.003%
53	10.877	3010	3018	3025	rVB2	598	792	0.12%	0.013%
54	11.009	3056	3059	3064	rVB2	204	191	0.03%	0.003%
55	11.135	3094	3098	3099	rBV	293	187	0.03%	0.003%
56	11.154	3099	3104	3115	rVB2	1856	2344	0.35%	0.037%
57	11.311	3149	3153	3155	rBV2	297	210	0.03%	0.003%
58	11.392	3171	3178	3180	rBV3	555	568	0.08%	0.009%
59	11.424	3180	3188	3196	rVV4	5986	9054	1.34%	0.143%
60	11.485	3196	3207	3230	rVV2	296072	521718	77.10%	8.234%
61	11.639	3248	3255	3259	rVB2	555	656	0.10%	0.010%
62	11.668	3259	3264	3272	rVB3	552	692	0.10%	0.011%
63	11.755	3285	3291	3299	rBV4	980	1685	0.25%	0.027%
64	11.861	3311	3324	3343	rBV	367853	580252	85.75%	9.158%
65	11.961	3353	3355	3362	rVB2	517	513	0.08%	0.008%
66	12.025	3371	3375	3381	rVB3	639	698	0.10%	0.011%
67	12.151	3411	3414	3417	rBV	207	165	0.02%	0.003%
68	12.250	3438	3445	3446	rBV2	1600	1135	0.17%	0.018%
69	12.482	3505	3517	3527	rBV2	3259	5802	0.86%	0.092%
70	12.655	3563	3571	3577	rBV	1100	1579	0.23%	0.025%
71	12.707	3580	3587	3599	rVB	2216	2789	0.41%	0.044%

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Integration Parameters: LSCINT.P

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72	12.839	3624	3628	3629	rBV2	636	415	0.06%	0.007%
73	12.884	3636	3642	3646	rBV	544	640	0.09%	0.010%
74	12.903	3646	3648	3654	rVB2	355	287	0.04%	0.005%
75	12.971	3665	3669	3675	rBV	152	206	0.03%	0.003%
76	13.125	3712	3717	3723	rBV4	912	958	0.14%	0.015%
77	13.241	3749	3753	3757	rBV	214	214	0.03%	0.003%
78	13.511	3832	3837	3843	rBV2	585	737	0.11%	0.012%
79	13.749	3906	3911	3913	rBV2	747	626	0.09%	0.010%
80	13.942	3968	3971	3973	rBV2	231	164	0.02%	0.003%
81	14.276	4066	4075	4085	rVB2	4010	6307	0.93%	0.100%
82	14.479	4132	4138	4145	rBV4	1185	1324	0.20%	0.021%
83	14.562	4160	4164	4166	rBV2	219	190	0.03%	0.003%
84	14.610	4175	4179	4182	rBV2	405	331	0.05%	0.005%
85	14.639	4185	4188	4190	rBV2	237	161	0.02%	0.003%
86	14.787	4225	4234	4240	rBV3	11071	15415	2.28%	0.243%
87	14.832	4241	4248	4259	rVV	18908	28547	4.22%	0.451%
88	14.890	4262	4266	4274	rVB4	3855	4522	0.67%	0.071%
89	15.012	4295	4304	4316	rBV4	15766	27766	4.10%	0.438%
90	15.089	4318	4328	4339	rVB	16148	24141	3.57%	0.381%
91	15.179	4349	4356	4365	rBV2	6644	9067	1.34%	0.143%
92	15.610	4480	4490	4506	rBV	35806	59982	8.86%	0.947%
93	15.880	4566	4574	4586	rBV	3620	5843	0.86%	0.092%
94	16.089	4636	4639	4645	rVB3	1268	1158	0.17%	0.018%
95	16.482	4756	4761	4768	rVB3	2102	2559	0.38%	0.040%
96	16.552	4771	4783	4796	rBV	452209	670700	99.12%	10.586%
97	16.639	4803	4810	4819	rVB5	3841	5310	0.78%	0.084%
98	16.703	4821	4830	4842	rVB2	23230	35430	5.24%	0.559%
99	17.282	5004	5010	5019	rVB3	5194	6962	1.03%	0.110%
100	17.488	5065	5074	5084	rBV4	15373	24967	3.69%	0.394%

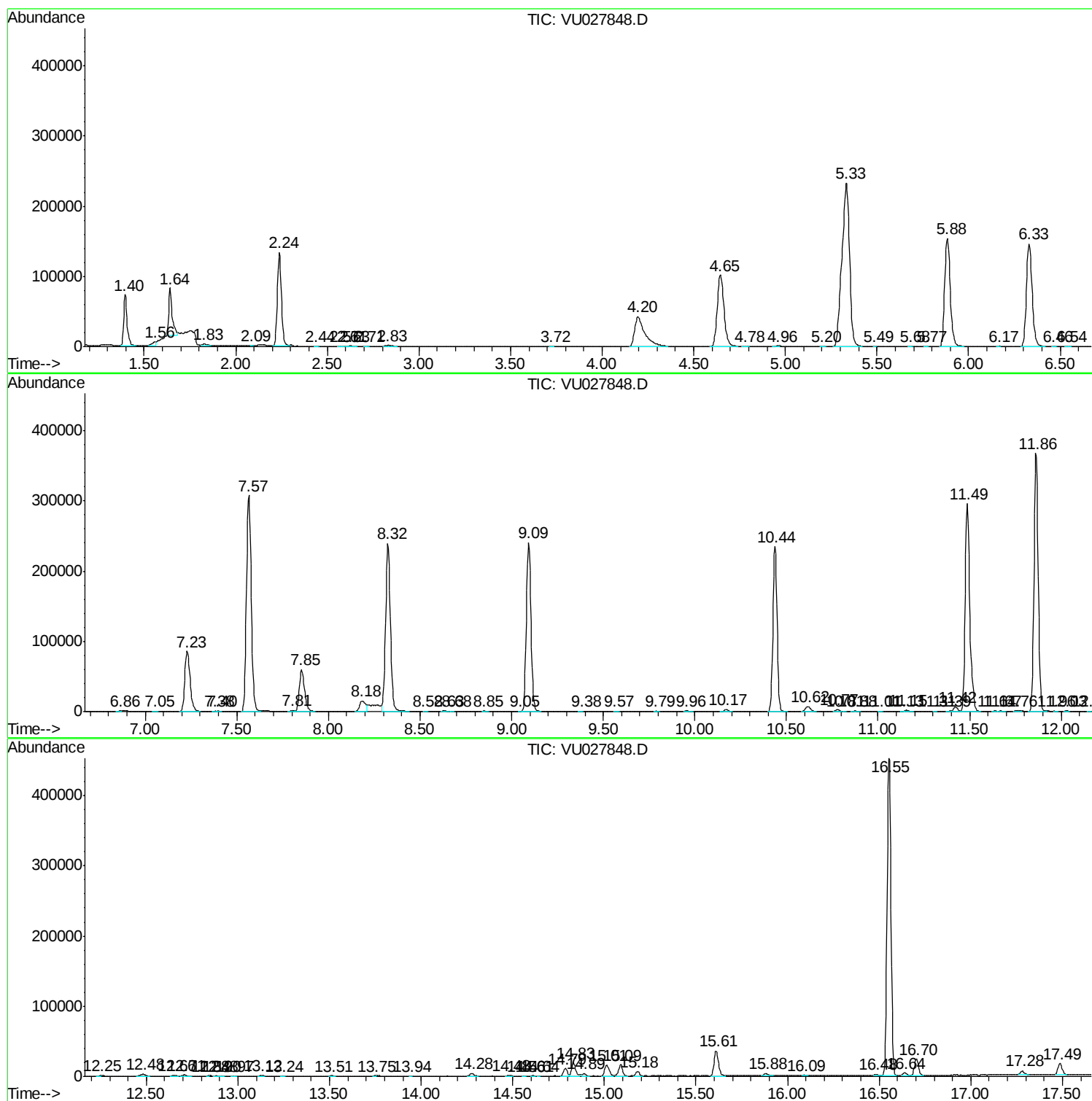
Sum of corrected areas: 6335814

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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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 Peak Number 1 (DEL) Alkane: Cyclic14.83 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	2.74 ug/L	28547	1,4-Dichlorobenzene-d4	11.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		2-Butyl-1-decene	196 C14H28	051655-65-3 94
2		Cyclobutanone, 3,3-dimethyl-	98 C6H10O	001192-33-2 72
3		Cyclobutane, 1,1-dimethyl-2-octyl-	196 C14H28	062338-30-1 64
4		Cyclopropane, 1-methyl-2-(1-meth...	140 C10H20	062238-06-6 64
5		1-Pentene, 2,4-dimethyl-	98 C7H14	002213-32-3 59

 Peak Number 2 (DEL) Alkane: Cyclic15.01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.01	2.66 ug/L	27766	1,4-Dichlorobenzene-d4	11.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Tridecane, 3-methylene-	196 C14H28	019780-34-8 83
2		Undecane, 3-methylene-	168 C12H24	071138-64-2 74
3		Nonane, 3-methylene-	140 C10H20	051655-64-2 59
4		2-Cyclohexen-1-ol	98 C6H10O	000822-67-3 50
5		Hexanal, 3-methyl-	114 C7H14O	019269-28-4 40

 Peak Number 3 Biphenyl Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.61	5.75 ug/L	59982	1,4-Dichlorobenzene-d4	11.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Biphenyl	154 C12H10	000092-52-4 95
2		Biphenyl	154 C12H10	000092-52-4 94
3		Biphenyl	154 C12H10	000092-52-4 93
4		Biphenyl	154 C12H10	000092-52-4 76
5		Naphthalene, 2-ethenyl-	154 C12H10	000827-54-3 72

 Peak Number 4 Butylated Hydroxytoluene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
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16.55	64.28 ug/L	670700	1,4-Dichlorobenzene-d4	11.49	
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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.70	3.40 ug/L	35430	1,4-Dichlorobenzene-d4	11.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1'-Biphenyl, 4-chloro-	188	C12H9Cl	002051-62-9	93
2	1,1'-Biphenyl, 2-chloro-	188	C12H9Cl	002051-60-7	93
3	1,1'-Biphenyl, 4-chloro-	188	C12H9Cl	002051-62-9	93
4	1,1'-Biphenyl, 4-chloro-	188	C12H9Cl	002051-62-9	93
5	1,1'-Biphenyl, 2-chloro-	188	C12H9Cl	002051-60-7	91

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: Cyc...	14.83	2.7	ug/L	28547	3	11.49	521718	50.0
(DEL) Alkane: Cyc...	15.01	2.7	ug/L	27766	3	11.49	521718	50.0
Biphenyl	15.61	5.8	ug/L	59982	3	11.49	521718	50.0
Butylated Hydroxy...	16.55	64.3	ug/L	670700	3	11.49	521718	50.0
1,1'-Biphenyl, 4-...	16.70	3.4	ug/L	35430	3	11.49	521718	50.0