

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU083118\
 Data File : VU026489.D
 Acq On : 31 Aug 2018 10:56
 Operator : MD/SY
 Sample : J4649-04
 Misc : 5.33g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GAB89

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\SOMULM082918WMA.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	1.085	140	154	169	rBV	214264	245131	31.66%	3.829%
2	1.284	211	216	224	rVB2	4393	4524	0.58%	0.071%
3	1.397	244	251	267	rBV	100440	102429	13.23%	1.600%
4	1.677	329	338	356	rVB	80454	108004	13.95%	1.687%
5	2.271	512	523	535	rBV	185920	278365	35.95%	4.348%
6	2.471	582	585	592	rBV2	461	513	0.07%	0.008%
7	2.561	610	613	615	rBV2	198	126	0.02%	0.002%
8	2.619	623	631	637	rBV	301	528	0.07%	0.008%
9	2.699	650	656	663	rVB2	772	1176	0.15%	0.018%
10	2.841	692	700	708	rBV3	643	1174	0.15%	0.018%
11	3.014	751	754	758	rVV	213	142	0.02%	0.002%
12	3.043	761	763	767	rVB	162	126	0.02%	0.002%
13	3.342	850	856	857	rBV	157	181	0.02%	0.003%
14	3.384	867	869	873	rVB2	380	315	0.04%	0.005%
15	3.406	873	876	878	rBV	261	151	0.02%	0.002%
16	3.706	963	969	974	rBV	174	291	0.04%	0.005%
17	3.751	978	983	986	rBV	180	233	0.03%	0.004%
18	3.931	1035	1039	1040	rBV	208	161	0.02%	0.003%
19	4.114	1094	1096	1099	rVB	247	139	0.02%	0.002%
20	4.178	1099	1116	1150	rBV	66598	182302	23.55%	2.848%
21	4.390	1177	1182	1183	rBV	266	185	0.02%	0.003%
22	4.651	1245	1263	1288	rVV2	119288	308000	39.78%	4.811%
23	4.738	1288	1290	1294	rVB2	293	174	0.02%	0.003%
24	4.786	1299	1305	1311	rVB2	352	538	0.07%	0.008%
25	4.821	1311	1316	1320	rBV2	285	357	0.05%	0.006%
26	4.841	1320	1322	1327	rVB	169	154	0.02%	0.002%
27	4.882	1330	1335	1339	rBV2	296	328	0.04%	0.005%
28	5.001	1370	1372	1375	rVB	243	136	0.02%	0.002%
29	5.024	1375	1379	1382	rBB	146	148	0.02%	0.002%
30	5.342	1453	1478	1505	rBV2	262630	774263	100.00%	12.094%
31	5.458	1511	1514	1517	rBV2	140	150	0.02%	0.002%
32	5.513	1528	1531	1535	rBB	147	143	0.02%	0.002%
33	5.596	1555	1557	1561	rBV	149	150	0.02%	0.002%
34	5.641	1565	1571	1574	rBV	183	250	0.03%	0.004%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\U083118\
 Data File : VU026489.D
 Acq On : 31 Aug 2018 10:56
 Operator : MD/SY
 Sample : J4649-04
 Misc : 5.33q/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GAB89

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\SOMULM082918WMA.M
 Title : VOC Analysis

35	5.754	1601	1606	1609	rVV2	215	247	0.03%	0.004%
36	5.889	1632	1648	1673	rBV	259043	499813	64.55%	7.807%
37	6.004	1681	1684	1687	rVB2	174	124	0.02%	0.002%
38	6.101	1708	1714	1716	rBB	175	193	0.02%	0.003%
39	6.191	1740	1742	1744	rBV	274	151	0.02%	0.002%
40	6.239	1753	1757	1760	rBV	145	170	0.02%	0.003%
41	6.268	1764	1766	1769	rVV2	203	144	0.02%	0.002%
42	6.332	1772	1786	1806	rBV	182373	362555	46.83%	5.663%
43	6.458	1822	1825	1829	rBV	211	247	0.03%	0.004%
44	6.545	1848	1852	1866	rVB	228	399	0.05%	0.006%
45	6.676	1890	1893	1895	rBV	149	129	0.02%	0.002%
46	6.776	1921	1924	1928	rBB	159	168	0.02%	0.003%
47	6.802	1929	1932	1934	rBV	149	122	0.02%	0.002%
48	6.959	1975	1981	1983	rBV	156	211	0.03%	0.003%
49	7.107	2021	2027	2030	rBV	159	220	0.03%	0.003%
50	7.229	2052	2065	2088	rBV	102302	177885	22.97%	2.779%
51	7.307	2088	2089	2092	rVV	274	132	0.02%	0.002%
52	7.567	2155	2170	2190	rBV	365746	621974	80.33%	9.716%
53	7.850	2247	2258	2277	rBV	73695	122038	15.76%	1.906%
54	8.043	2315	2318	2322	rVB	188	123	0.02%	0.002%
55	8.184	2347	2362	2372	rBV2	25262	57172	7.38%	0.893%
56	8.313	2392	2402	2431	rVB	240125	408231	52.73%	6.377%
57	8.419	2432	2435	2437	rBV2	271	159	0.02%	0.002%
58	8.471	2442	2451	2463	rVV4	4571	7208	0.93%	0.113%
59	8.676	2512	2515	2517	rVB2	261	141	0.02%	0.002%
60	8.699	2517	2522	2528	rBV	134	167	0.02%	0.003%
61	9.091	2630	2644	2667	rBV	365739	592091	76.47%	9.249%
62	9.252	2686	2694	2707	rVV2	837	1433	0.19%	0.022%
63	9.377	2725	2733	2744	rVB	3878	5643	0.73%	0.088%
64	9.782	2851	2859	2869	rBV5	2223	3157	0.41%	0.049%
65	10.043	2936	2940	2946	rBV	121	139	0.02%	0.002%
66	10.316	3020	3025	3028	rBV3	512	449	0.06%	0.007%
67	10.432	3049	3061	3076	rBV	255042	402820	52.03%	6.292%
68	10.615	3106	3118	3131	rBV	7873	14609	1.89%	0.228%
69	10.847	3188	3190	3193	rVB2	222	122	0.02%	0.002%
70	10.872	3194	3198	3204	rBV2	328	314	0.04%	0.005%
71	11.072	3256	3260	3265	rVB2	173	185	0.02%	0.003%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU083118\
 Data File : VU026489.D
 Acq On : 31 Aug 2018 10:56
 Operator : MD/SY
 Sample : J4649-04
 Misc : 5.33g/5mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GAB89

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\SOMULM082918WMA.M
 Title : VOC Analysis

72	11.171	3289	3291	3295	rBV	275	143	0.02%	0.002%
73	11.483	3376	3388	3405	rBV	338784	531853	68.69%	8.308%
74	11.583	3415	3419	3422	rBV2	251	183	0.02%	0.003%
75	11.798	3483	3486	3489	rVB2	217	140	0.02%	0.002%
76	11.863	3493	3506	3527	rBV	357054	567106	73.24%	8.858%
77	12.078	3570	3573	3577	rVB	179	123	0.02%	0.002%
78	12.133	3586	3590	3593	rBV2	175	145	0.02%	0.002%
79	12.213	3611	3615	3619	rVB2	257	223	0.03%	0.003%
80	12.332	3648	3652	3658	rVB	205	253	0.03%	0.004%
81	12.483	3689	3699	3709	rVB2	1686	3071	0.40%	0.048%
82	12.532	3709	3714	3718	rBV2	172	187	0.02%	0.003%
83	12.583	3727	3730	3732	rBV	309	198	0.03%	0.003%
84	12.663	3752	3755	3758	rBV2	270	149	0.02%	0.002%
85	12.779	3789	3791	3793	rVV	223	126	0.02%	0.002%
86	12.995	3855	3858	3861	rBV	344	186	0.02%	0.003%
87	13.178	3912	3915	3919	rVB	244	223	0.03%	0.003%
88	13.361	3971	3972	3975	rBV	214	131	0.02%	0.002%
89	13.432	3991	3994	3995	rBV2	266	159	0.02%	0.002%
90	13.464	4002	4004	4006	rBV2	288	142	0.02%	0.002%
91	13.512	4016	4019	4023	rBV	209	140	0.02%	0.002%
92	13.599	4043	4046	4052	rBV	192	180	0.02%	0.003%
93	13.631	4052	4056	4058	rVV	208	150	0.02%	0.002%
94	13.763	4093	4097	4098	rBV	243	134	0.02%	0.002%
95	13.811	4108	4112	4114	rBV2	198	141	0.02%	0.002%
96	13.872	4127	4131	4136	rVB3	262	274	0.04%	0.004%
97	14.120	4205	4208	4210	rBV	274	203	0.03%	0.003%
98	14.216	4236	4238	4241	rBV2	226	190	0.02%	0.003%
99	14.281	4248	4258	4269	rBV2	2040	3343	0.43%	0.052%
100	16.502	4947	4949	4952	rBV2	474	277	0.04%	0.004%

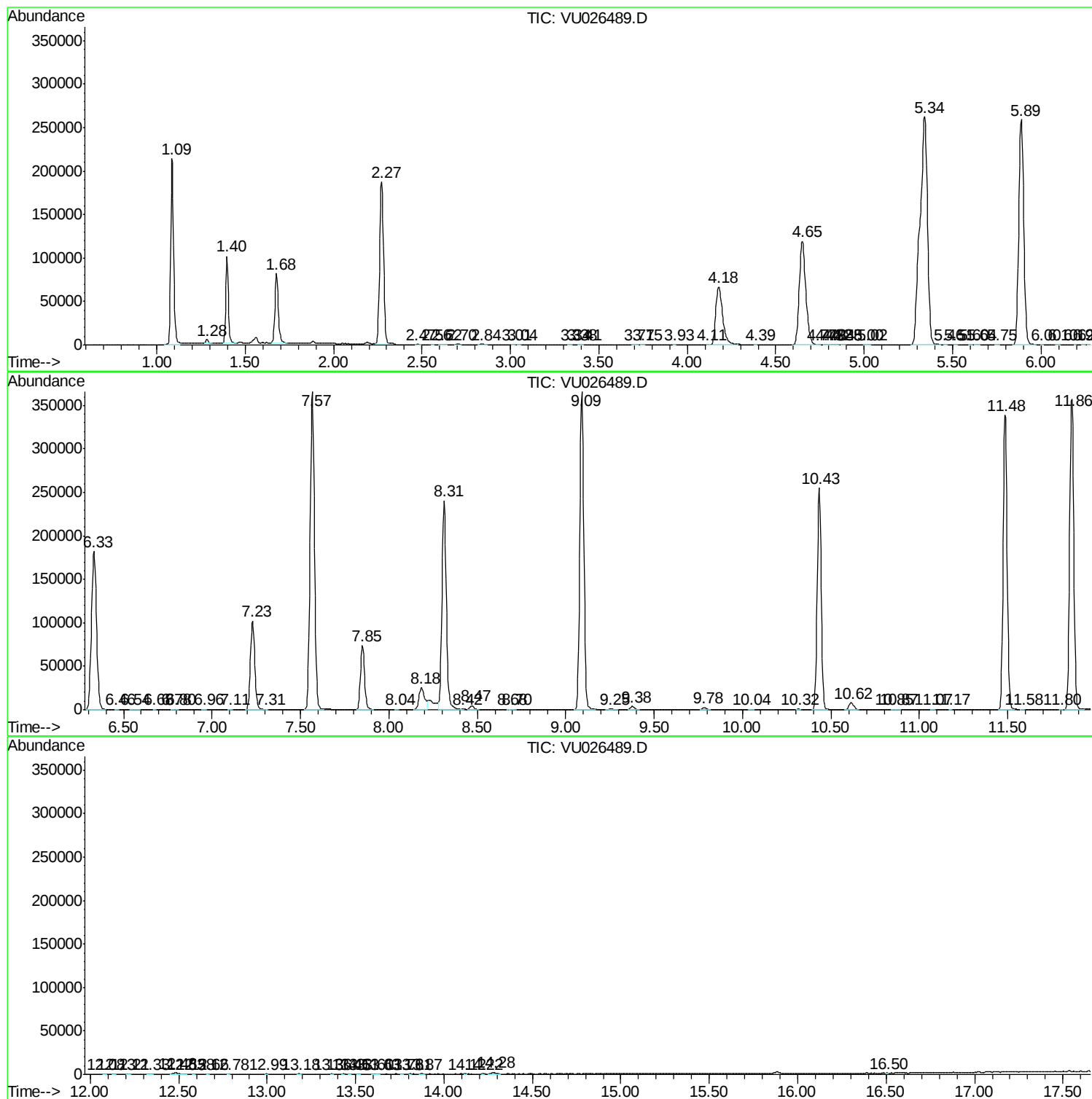
Sum of corrected areas: 6401845

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU083118\
Data File : VU026489.D
Acq On : 31 Aug 2018 10:56
Operator : MD/SY
Sample : J4649-04
Misc : 5.33q/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GAB89

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082918WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU083118\
Data File : VU026489.D
Acq On : 31 Aug 2018 10:56
Operator : MD/SY
Sample : J4649-04
Misc : 5.33g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GAB89

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082918WMA.M
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU083118\
Data File : VU026489.D
Acq On : 31 Aug 2018 10:56
Operator : MD/SY
Sample : J4649-04
Misc : 5.33g/5mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GAB89

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082918WMA.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