

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU033123\
 Data File : VU053493.D
 Acq On : 31 Mar 2023 15:50
 Operator : JC/MD
 Sample : VU0331MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK061

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
 Title : VOC Analysis

Signal : TIC: VU053493.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	72	80	91	rBV	158307	174989	17.74%	2.202%
2	1.909	169	177	192	rVB	117103	155481	15.76%	1.956%
3	2.565	369	381	407	rVB	232814	377194	38.24%	4.746%
4	2.723	428	430	434	rVB2	479	314	0.03%	0.004%
5	2.790	443	451	462	rVB2	3491	5464	0.55%	0.069%
6	3.044	521	530	540	rBV6	1907	3513	0.36%	0.044%
7	3.170	566	569	571	rBV2	371	266	0.03%	0.003%
8	3.353	618	626	635	rBV5	1756	3248	0.33%	0.041%
9	3.851	779	781	784	rBV	297	183	0.02%	0.002%
10	4.205	889	891	895	rVB2	269	164	0.02%	0.002%
11	4.231	895	899	902	rBV	243	190	0.02%	0.002%
12	4.311	923	924	925	rBV	127	34	0.00%	0.000%
13	4.494	976	981	984	rBV	461	388	0.04%	0.005%
14	4.613	1007	1018	1049	rBV	75402	183865	18.64%	2.313%
15	5.057	1141	1156	1179	rBV	187678	412770	41.85%	5.193%
16	5.340	1241	1244	1248	rBV2	165	132	0.01%	0.002%
17	5.372	1251	1254	1255	rBV	462	284	0.03%	0.004%
18	5.420	1265	1269	1274	rVB2	258	232	0.02%	0.003%
19	5.616	1328	1330	1333	rBV2	157	97	0.01%	0.001%
20	5.649	1338	1340	1341	rBV	173	93	0.01%	0.001%
21	5.719	1341	1362	1385	rBV2	360817	986381	100.00%	12.410%
22	5.983	1442	1444	1450	rVB2	216	168	0.02%	0.002%
23	6.086	1473	1476	1478	rBV	170	89	0.01%	0.001%
24	6.121	1484	1487	1489	rBV3	310	202	0.02%	0.003%
25	6.189	1504	1508	1512	rBV2	330	252	0.03%	0.003%
26	6.243	1512	1525	1547	rBV	312988	598965	60.72%	7.536%
27	6.468	1591	1595	1599	rBV	312	352	0.04%	0.004%
28	6.529	1604	1614	1626	rVB9	5988	11785	1.19%	0.148%
29	6.575	1626	1628	1630	rBV	182	108	0.01%	0.001%
30	6.687	1649	1663	1680	rBV	222490	434174	44.02%	5.463%
31	6.867	1716	1719	1721	rBV	156	90	0.01%	0.001%
32	6.922	1732	1736	1737	rBV2	250	145	0.01%	0.002%
33	7.021	1765	1767	1769	rBV	218	107	0.01%	0.001%
34	7.102	1789	1792	1795	rBV2	219	187	0.02%	0.002%
35	7.272	1842	1845	1848	rVB2	228	183	0.02%	0.002%
36	7.324	1859	1861	1866	rVB	268	160	0.02%	0.002%

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
 Title : VOC Analysis

37	7.414	1885	1889	1891	rBV	338	223	0.02%	0.003%
38	7.562	1921	1935	1958	rBV	129591	235078	23.83%	2.958%
39	7.726	1984	1986	1988	rBV2	277	129	0.01%	0.002%
40	7.755	1993	1995	1997	rVB2	222	86	0.01%	0.001%
41	7.825	2014	2017	2020	rBV2	260	180	0.02%	0.002%
42	7.893	2025	2038	2059	rBV	491920	851609	86.34%	10.714%
43	8.115	2104	2107	2112	rBV	195	161	0.02%	0.002%
44	8.176	2115	2126	2145	rVV	91019	157165	15.93%	1.977%
45	8.275	2155	2157	2159	rBV	229	92	0.01%	0.001%
46	8.301	2163	2165	2170	rVB	256	121	0.01%	0.002%
47	8.353	2177	2181	2190	rBV2	311	560	0.06%	0.007%
48	8.398	2190	2195	2198	rVV3	295	264	0.03%	0.003%
49	8.510	2227	2230	2233	rVB2	206	138	0.01%	0.002%
50	8.549	2236	2242	2251	rBV6	2448	3852	0.39%	0.048%
51	8.629	2255	2267	2294	rBV	223140	415450	42.12%	5.227%
52	8.896	2349	2350	2351	rBV	149	35	0.00%	0.000%
53	9.073	2398	2405	2406	rBV2	261	270	0.03%	0.003%
54	9.169	2432	2435	2438	rBV	324	141	0.01%	0.002%
55	9.285	2468	2471	2472	rBV	156	89	0.01%	0.001%
56	9.304	2475	2477	2480	rVB	273	112	0.01%	0.001%
57	9.414	2495	2511	2542	rBV	435525	722064	73.20%	9.085%
58	9.697	2590	2599	2606	rBV2	2163	3487	0.35%	0.044%
59	9.793	2627	2629	2634	rBV	195	142	0.01%	0.002%
60	10.108	2720	2727	2738	rVB5	2656	4765	0.48%	0.060%
61	10.295	2779	2785	2788	rBV2	377	368	0.04%	0.005%
62	10.330	2792	2796	2801	rBV2	241	238	0.02%	0.003%
63	10.751	2915	2927	2944	rBV	330085	516224	52.34%	6.495%
64	11.037	3014	3016	3019	rBV	197	122	0.01%	0.002%
65	11.086	3024	3031	3039	rBV4	1776	2687	0.27%	0.034%
66	11.205	3065	3068	3071	rVB	252	163	0.02%	0.002%
67	11.227	3071	3075	3076	rBV	163	124	0.01%	0.002%
68	11.414	3130	3133	3137	rBV	276	191	0.02%	0.002%
69	11.465	3143	3149	3159	rVB5	2879	4367	0.44%	0.055%
70	11.700	3219	3222	3225	rBV2	346	269	0.03%	0.003%
71	11.742	3228	3235	3243	rBV3	4465	6833	0.69%	0.086%
72	11.806	3244	3255	3288	rVV	467350	761587	77.21%	9.582%
73	12.047	3328	3330	3335	rBV2	239	179	0.02%	0.002%
74	12.086	3340	3342	3343	rBV2	252	108	0.01%	0.001%
75	12.188	3361	3374	3391	rBV	511852	828820	84.03%	10.428%
76	12.362	3426	3428	3430	rVB	180	74	0.01%	0.001%

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M

Title : VOC Analysis

77	12.375	3430	3432	3436	rBV2	315	237	0.02%	0.003%
78	12.497	3467	3470	3474	rVB	367	231	0.02%	0.003%
79	12.597	3499	3501	3502	rBV	148	47	0.00%	0.001%
80	12.719	3537	3539	3541	rBB	325	113	0.01%	0.001%
81	13.124	3662	3665	3667	rBV	358	200	0.02%	0.003%
82	13.221	3688	3695	3707	rVB2	6329	9576	0.97%	0.120%
83	13.266	3707	3709	3717	rVB3	352	334	0.03%	0.004%
84	13.298	3717	3719	3724	rVB	350	222	0.02%	0.003%
85	13.336	3728	3731	3732	rBV	322	183	0.02%	0.002%
86	13.462	3767	3770	3776	rVB2	424	342	0.03%	0.004%
87	13.838	3880	3887	3902	rVB3	11167	17185	1.74%	0.216%
88	14.085	3956	3964	3983	rVB	18224	31005	3.14%	0.390%
89	14.327	4031	4039	4048	rBV2	11487	17719	1.80%	0.223%

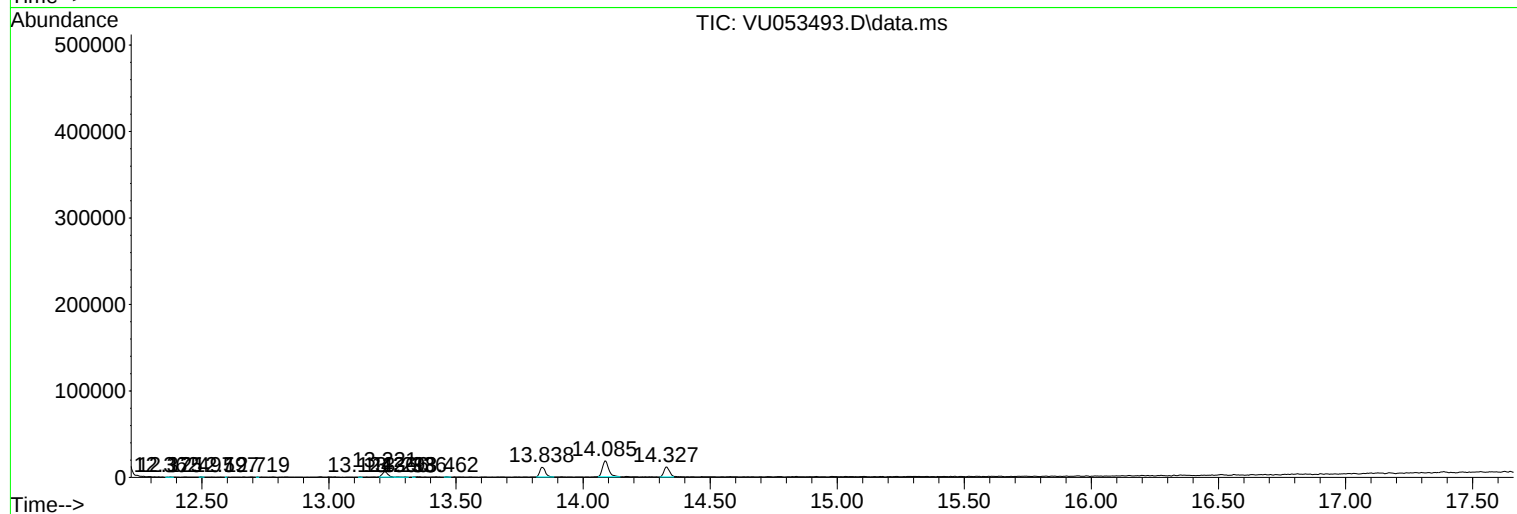
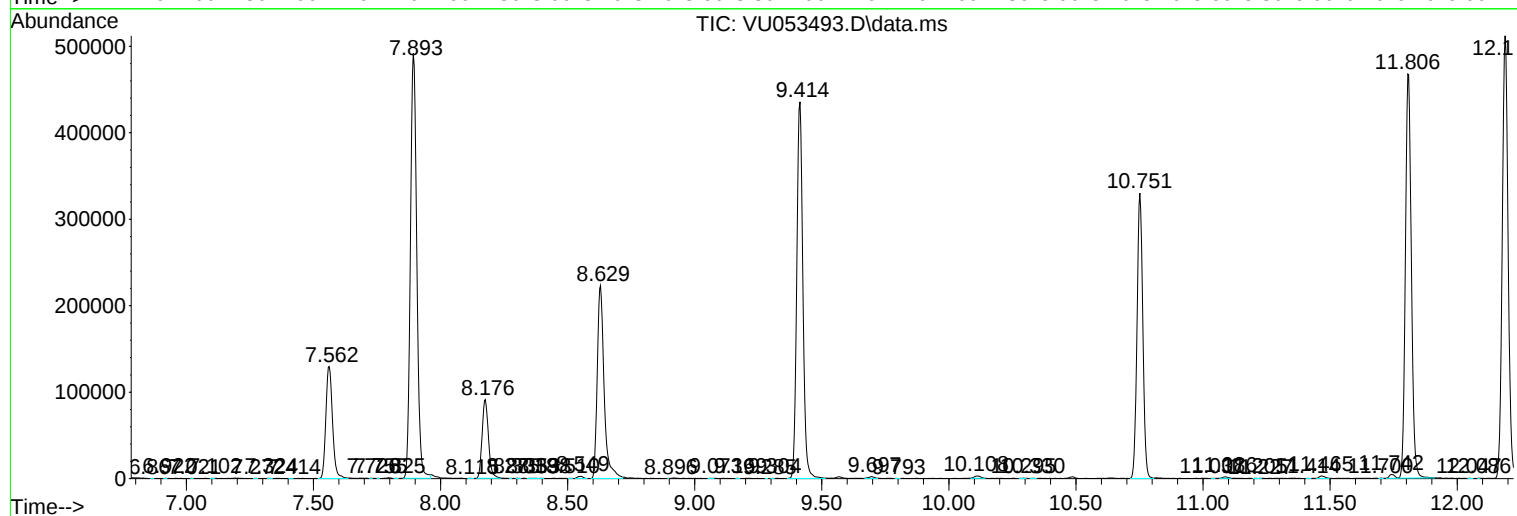
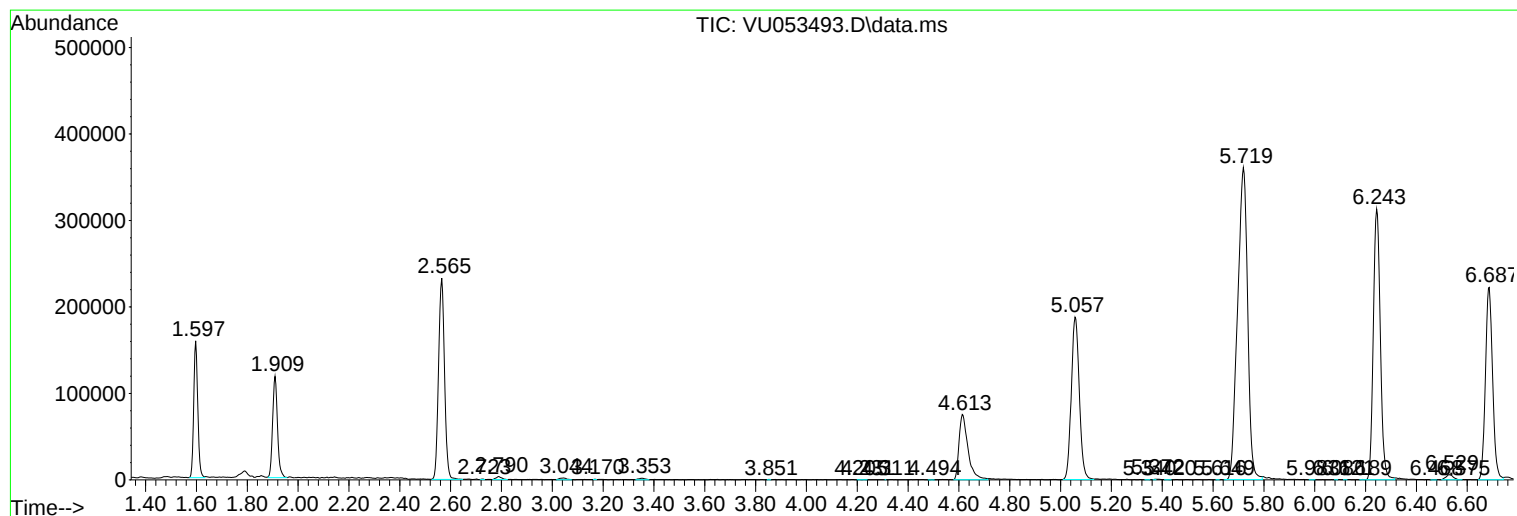
Sum of corrected areas: 7948210

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

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Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM033123WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
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