

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121423\
 Data File : VV033343.D
 Acq On : 14 Dec 2023 18:18
 Operator : SY/MD
 Sample : 05794-10
 Misc : 4.80g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BH3Q5

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_V\Method\SFAMVLM120123WMA.M
 Title : VOC Analysis

Signal : TIC: VV033343.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.060	304	317	340	rBV	176366	259037	29.40%	6.367%
2	2.159	345	348	350	rBB	246	114	0.01%	0.003%
3	2.275	381	384	387	rBB2	259	169	0.02%	0.004%
4	2.323	396	399	403	rBB2	258	193	0.02%	0.005%
5	2.384	415	418	421	rBV2	244	218	0.02%	0.005%
6	2.449	431	438	446	rBV4	1278	1887	0.21%	0.046%
7	2.539	462	466	467	rBV	474	368	0.04%	0.009%
8	2.902	577	579	582	rBB	247	138	0.02%	0.003%
9	3.092	636	638	640	rBV	234	127	0.01%	0.003%
10	3.127	648	649	655	rBB	126	135	0.02%	0.003%
11	3.156	656	658	663	rBB	142	143	0.02%	0.004%
12	3.709	826	830	832	rBB	150	124	0.01%	0.003%
13	3.783	844	853	892	rVV	44462	122881	13.94%	3.021%
14	4.568	1094	1097	1098	rBV	362	183	0.02%	0.004%
15	4.626	1111	1115	1117	rBB	250	175	0.02%	0.004%
16	4.651	1121	1123	1126	rBV	338	211	0.02%	0.005%
17	4.706	1134	1140	1142	rBV	220	251	0.03%	0.006%
18	4.957	1199	1218	1249	rBV2	329670	881200	100.00%	21.661%
19	5.465	1373	1376	1378	rBV2	406	300	0.03%	0.007%
20	5.532	1383	1397	1429	rBV2	250844	518839	58.88%	12.754%
21	5.989	1526	1539	1558	rBV2	179929	367845	41.74%	9.042%
22	6.198	1600	1604	1606	rBB	361	188	0.02%	0.005%
23	6.214	1607	1609	1610	rBV	243	125	0.01%	0.003%
24	6.265	1623	1625	1629	rBB	256	156	0.02%	0.004%
25	6.294	1630	1634	1637	rBV	212	202	0.02%	0.005%
26	6.333	1642	1646	1649	rBV2	267	196	0.02%	0.005%
27	6.558	1713	1716	1719	rBB	174	139	0.02%	0.003%
28	6.638	1736	1741	1746	rBB2	300	309	0.04%	0.008%
29	6.703	1758	1761	1765	rBB	135	138	0.02%	0.003%
30	6.912	1816	1826	1854	rBV	108436	200339	22.73%	4.925%
31	7.130	1892	1894	1896	rBV	338	154	0.02%	0.004%
32	7.805	2102	2104	2105	rBV	256	122	0.01%	0.003%
33	7.850	2116	2118	2119	rBV	365	172	0.02%	0.004%
34	8.024	2163	2172	2208	rBV	163585	310874	35.28%	7.642%
35	8.567	2340	2341	2344	rBV	340	204	0.02%	0.005%
36	8.625	2356	2359	2364	rBB2	278	254	0.03%	0.006%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
 Title : VOC Analysis

37	8.783	2398	2408	2434	rBV	399323	659826	74.88%	16.219%
38	9.059	2492	2494	2498	rBB	186	114	0.01%	0.003%
39	9.124	2511	2514	2517	rBB	258	182	0.02%	0.004%
40	9.162	2522	2526	2528	rBV	304	206	0.02%	0.005%
41	9.272	2557	2560	2565	rBB	268	197	0.02%	0.005%
42	9.313	2570	2573	2575	rBB	318	152	0.02%	0.004%
43	9.381	2590	2594	2598	rBB2	268	242	0.03%	0.006%
44	9.452	2612	2616	2619	rBB2	300	238	0.03%	0.006%
45	9.574	2651	2654	2658	rBB2	349	167	0.02%	0.004%
46	9.654	2677	2679	2681	rBV	275	148	0.02%	0.004%
47	9.731	2700	2703	2706	rBV	126	132	0.01%	0.003%
48	9.847	2737	2739	2742	rBB2	275	145	0.02%	0.004%
49	9.866	2742	2745	2748	rBB	132	115	0.01%	0.003%
50	9.944	2766	2769	2771	rBB	245	160	0.02%	0.004%
51	9.976	2777	2779	2781	rBV	159	110	0.01%	0.003%
52	10.014	2789	2791	2793	rBV	196	122	0.01%	0.003%
53	10.329	2879	2889	2898	rBB5	2967	5061	0.57%	0.124%
54	10.432	2919	2921	2924	rBB	317	190	0.02%	0.005%
55	10.503	2940	2943	2945	rBB	276	171	0.02%	0.004%
56	10.587	2966	2969	2974	rBB2	394	308	0.03%	0.008%
57	10.609	2974	2976	2980	rBB	203	163	0.02%	0.004%
58	10.680	2996	2998	3000	rBV	255	167	0.02%	0.004%
59	10.789	3028	3032	3034	rBV2	362	253	0.03%	0.006%
60	10.847	3047	3050	3054	rBB2	230	192	0.02%	0.005%
61	11.056	3112	3115	3117	rBB2	246	140	0.02%	0.003%
62	11.075	3118	3121	3123	rBV2	388	203	0.02%	0.005%
63	11.185	3140	3155	3178	rBV	471664	721190	81.84%	17.728%
64	11.436	3229	3233	3237	rBV2	252	284	0.03%	0.007%
65	11.464	3240	3242	3247	rBB	152	153	0.02%	0.004%
66	11.500	3250	3253	3256	rBB2	277	197	0.02%	0.005%
67	11.519	3257	3259	3260	rBV2	265	106	0.01%	0.003%
68	11.764	3332	3335	3339	rBB	371	188	0.02%	0.005%
69	11.789	3340	3343	3346	rBB	371	198	0.02%	0.005%
70	11.863	3364	3366	3371	rBB	154	146	0.02%	0.004%
71	11.902	3376	3378	3381	rBB2	254	180	0.02%	0.004%
72	12.072	3428	3431	3433	rBB	270	127	0.01%	0.003%
73	12.104	3438	3441	3443	rBV	209	161	0.02%	0.004%
74	12.194	3462	3469	3480	rBB3	1785	2739	0.31%	0.067%
75	12.333	3509	3512	3515	rBB	155	123	0.01%	0.003%
76	12.352	3516	3518	3520	rBB	277	145	0.02%	0.004%

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 Title : VOC Analysis

77	12.403	3530	3534	3535	rBV	285	186	0.02%	0.005%
78	12.481	3555	3558	3560	rBV	265	188	0.02%	0.005%
79	12.538	3572	3576	3578	rBV	265	195	0.02%	0.005%
80	12.606	3595	3597	3599	rBV	264	150	0.02%	0.004%
81	12.644	3607	3609	3610	rBV	252	117	0.01%	0.003%
82	12.821	3661	3664	3666	rBV	148	120	0.01%	0.003%
83	12.963	3705	3708	3711	rBB	227	111	0.01%	0.003%
84	12.982	3712	3714	3716	rBV2	250	139	0.02%	0.003%
85	13.075	3740	3743	3746	rBB	408	269	0.03%	0.007%
86	13.091	3747	3748	3757	rBV5	387	501	0.06%	0.012%
87	13.181	3774	3776	3778	rBB	273	147	0.02%	0.004%
88	13.233	3790	3792	3794	rBB	254	117	0.01%	0.003%
89	13.252	3795	3798	3801	rBB	247	178	0.02%	0.004%
90	13.342	3824	3826	3828	rBB	280	126	0.01%	0.003%
91	13.355	3828	3830	3833	rBB	274	144	0.02%	0.004%
92	13.371	3833	3835	3836	rBV	272	148	0.02%	0.004%
93	13.400	3840	3844	3845	rBV2	351	229	0.03%	0.006%
94	13.471	3859	3866	3869	rBB2	641	490	0.06%	0.012%
95	13.603	3905	3907	3911	rBV	250	190	0.02%	0.005%
96	13.654	3921	3923	3927	rBB	404	225	0.03%	0.006%
97	13.677	3927	3930	3932	rBV	512	279	0.03%	0.007%
98	13.744	3949	3951	3952	rBV	259	117	0.01%	0.003%
99	13.847	3981	3983	3986	rBV	574	334	0.04%	0.008%
100	13.905	3999	4001	4002	rBV	483	269	0.03%	0.007%

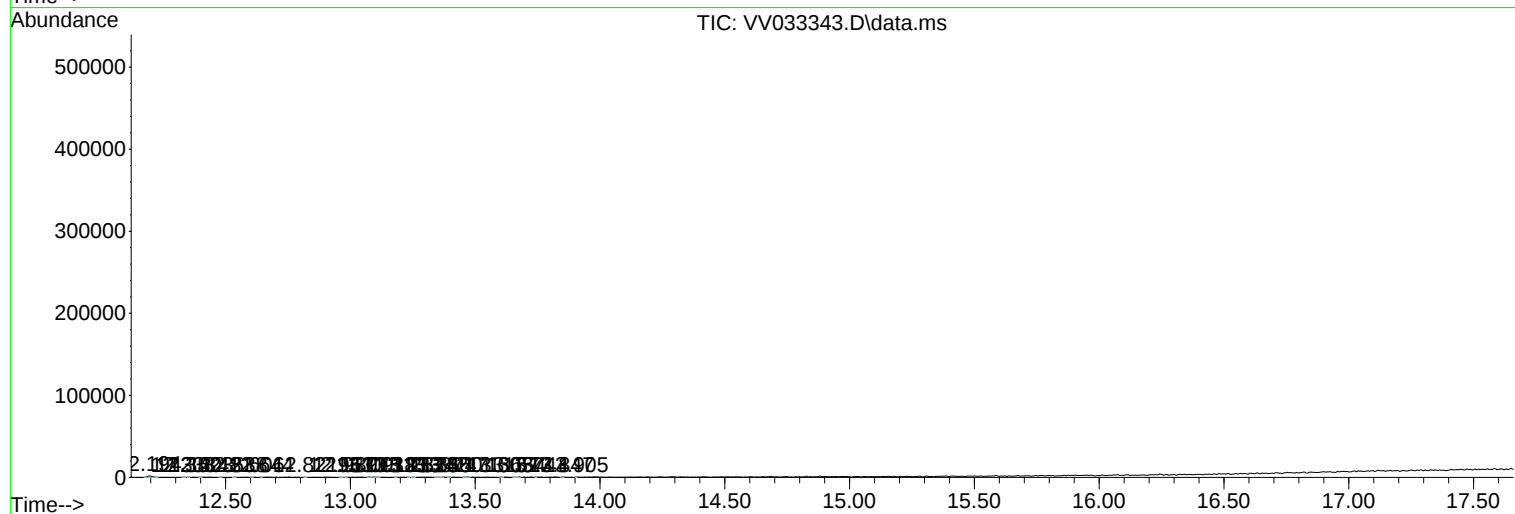
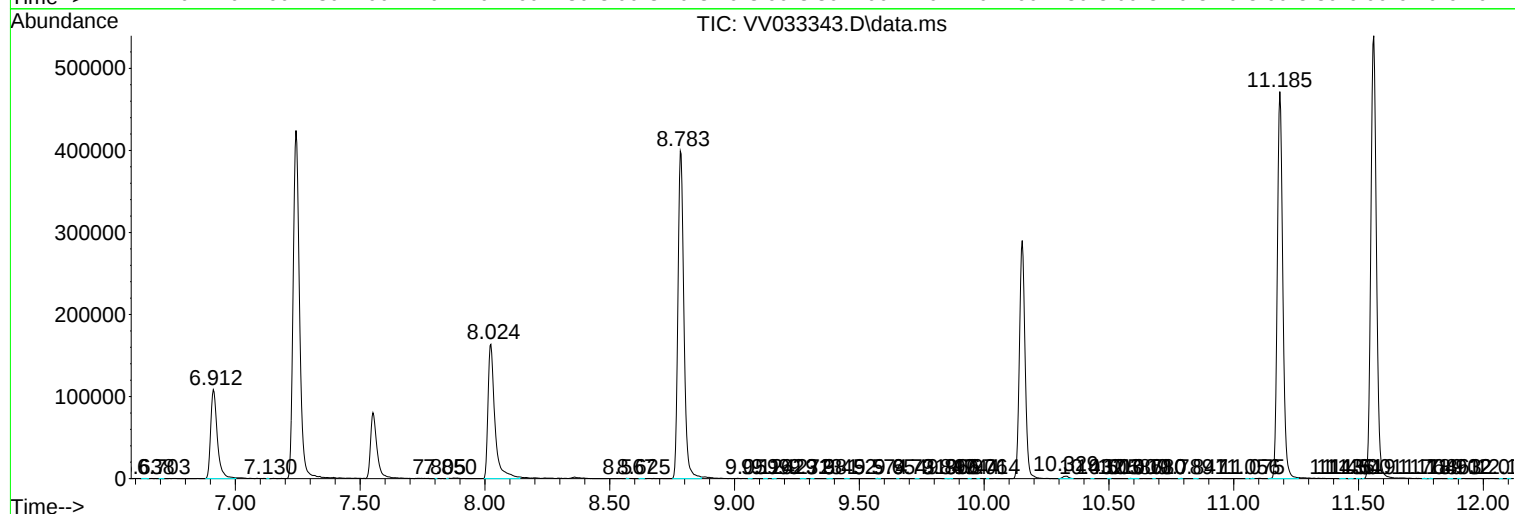
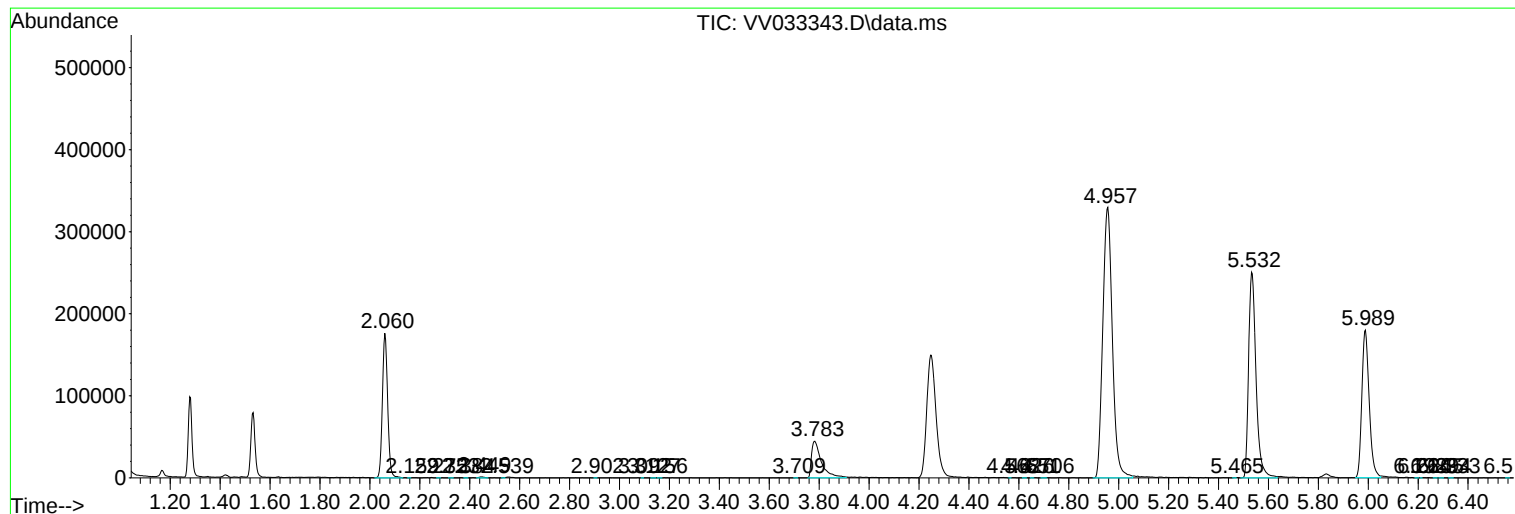
Sum of corrected areas: 4068120

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.M
Quant Title : VOC Analysis

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



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120123WMA.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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TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
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