

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV120224\
 Data File : VV038391.D
 Acq On : 02 Dec 2024 16:14
 Operator : SY/MD
 Sample : VV1202MBL01
 Misc : 5.00g/5mL/100ul/5ML/MSVOA_V/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VBLK255

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_V\Method\SFAMVLM120224WMA.M
 Title : VOC Analysis

Signal : TIC: VV038391.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.275	67	73	90	rVB	318341	346309	15.08%	2.005%
2	1.529	145	152	166	rVB	278990	327011	14.24%	1.893%
3	2.053	306	315	346	rVB	558895	845172	36.81%	4.893%
4	2.558	471	472	476	rVB2	964	378	0.02%	0.002%
5	2.670	505	507	509	rBV3	466	257	0.01%	0.001%
6	2.693	510	514	516	rBV2	1469	1395	0.06%	0.008%
7	2.735	525	527	532	rVB4	995	611	0.03%	0.004%
8	2.761	532	535	538	rBV3	645	476	0.02%	0.003%
9	3.066	627	630	633	rBV	491	386	0.02%	0.002%
10	3.130	648	650	654	rVB2	411	207	0.01%	0.001%
11	3.162	658	660	663	rBV3	588	391	0.02%	0.002%
12	3.182	663	666	668	rBV3	444	272	0.01%	0.002%
13	3.233	681	682	683	rBV	448	93	0.00%	0.001%
14	3.262	688	691	692	rBV2	413	225	0.01%	0.001%
15	3.301	700	703	709	rVB2	503	518	0.02%	0.003%
16	3.352	717	719	725	rVB2	622	589	0.03%	0.003%
17	3.387	725	730	732	rBV2	501	475	0.02%	0.003%
18	3.397	732	733	735	rBV	459	235	0.01%	0.001%
19	3.445	744	748	750	rBV4	785	708	0.03%	0.004%
20	3.500	760	765	766	rBV2	395	298	0.01%	0.002%
21	3.529	771	774	777	rVV2	477	309	0.01%	0.002%
22	3.548	777	780	785	rVB2	439	316	0.01%	0.002%
23	3.571	785	787	788	rBV	247	97	0.00%	0.001%
24	3.606	797	798	801	rVB2	304	123	0.01%	0.001%
25	3.658	808	814	816	rBV2	595	518	0.02%	0.003%
26	3.741	837	840	841	rBV2	196	94	0.00%	0.001%
27	3.783	844	853	892	rBV2	126043	392178	17.08%	2.270%
28	4.240	981	995	1026	rBV	355595	918546	40.01%	5.317%
29	4.947	1200	1215	1247	rBV2	871199	2296076	100.00%	13.292%
30	5.375	1346	1348	1351	rVB3	1108	648	0.03%	0.004%
31	5.526	1384	1395	1430	rBV	622683	1326096	57.75%	7.677%
32	5.979	1523	1536	1578	rBV	490593	1062939	46.29%	6.153%
33	6.407	1665	1669	1672	rBV3	801	586	0.03%	0.003%
34	6.526	1704	1706	1707	rBV2	476	177	0.01%	0.001%
35	6.551	1711	1714	1717	rBV2	730	517	0.02%	0.003%
36	6.690	1754	1757	1758	rBV2	784	421	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV120224\
 Data File : VV038391.D
 Acq On : 02 Dec 2024 16:14
 Operator : SY/MD
 Sample : VV1202MBL01
 Misc : 5.00g/5mL/100ul/5ML/MSVOA_V/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VBLK255

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_V\Method\SFAMVLM120224WMA.M
 Title : VOC Analysis

37	6.728	1767	1769	1771	rBV2	726	391	0.02%	0.002%
38	6.764	1775	1780	1783	rVV4	862	830	0.04%	0.005%
39	6.789	1786	1788	1791	rBV3	418	188	0.01%	0.001%
40	6.805	1791	1793	1795	rBV3	467	235	0.01%	0.001%
41	6.831	1799	1801	1802	rBV2	268	94	0.00%	0.001%
42	6.841	1802	1804	1805	rBV	450	194	0.01%	0.001%
43	6.905	1813	1824	1860	rBV	248980	511143	22.26%	2.959%
44	7.233	1916	1926	1964	rBV	1000391	1827709	79.60%	10.580%
45	7.545	2015	2023	2051	rBV2	168975	338879	14.76%	1.962%
46	8.018	2162	2170	2218	rBV	395380	872415	38.00%	5.050%
47	8.509	2318	2323	2326	rBV6	1604	1241	0.05%	0.007%
48	8.616	2354	2356	2359	rBV3	1007	521	0.02%	0.003%
49	8.725	2388	2390	2393	rBV3	533	277	0.01%	0.002%
50	8.776	2395	2406	2444	rBV	1017346	1726471	75.19%	9.994%
51	9.355	2580	2586	2588	rBV3	663	801	0.03%	0.005%
52	9.410	2601	2603	2605	rBV2	470	296	0.01%	0.002%
53	9.458	2617	2618	2620	rBV	340	145	0.01%	0.001%
54	9.468	2620	2621	2623	rBV	543	221	0.01%	0.001%
55	9.542	2641	2644	2646	rBV2	1181	641	0.03%	0.004%
56	9.628	2668	2671	2673	rBV2	1018	629	0.03%	0.004%
57	9.709	2694	2696	2698	rVB2	510	224	0.01%	0.001%
58	9.725	2699	2701	2703	rVB	387	140	0.01%	0.001%
59	9.744	2703	2707	2709	rBV2	820	478	0.02%	0.003%
60	9.812	2727	2728	2729	rBV2	248	58	0.00%	0.000%
61	9.828	2729	2733	2734	rBV	401	240	0.01%	0.001%
62	9.837	2734	2736	2740	rVB3	562	396	0.02%	0.002%
63	9.866	2740	2745	2746	rBV3	1203	1138	0.05%	0.007%
64	9.950	2768	2771	2776	rBV3	597	510	0.02%	0.003%
65	9.998	2784	2786	2789	rVB2	568	237	0.01%	0.001%
66	10.011	2789	2790	2792	rVB	680	236	0.01%	0.001%
67	10.027	2792	2795	2797	rBV3	928	483	0.02%	0.003%
68	10.037	2797	2798	2801	rBV2	557	258	0.01%	0.001%
69	10.085	2812	2813	2814	rBV	225	77	0.00%	0.000%
70	10.143	2819	2831	2859	rBV	673326	1098262	47.83%	6.358%
71	10.407	2910	2913	2916	rBV2	835	641	0.03%	0.004%
72	10.423	2916	2918	2920	rBV3	609	304	0.01%	0.002%
73	10.545	2954	2956	2960	rBV2	426	187	0.01%	0.001%
74	10.587	2967	2969	2971	rBV3	547	288	0.01%	0.002%
75	10.609	2974	2976	2978	rVB2	643	225	0.01%	0.001%
76	10.625	2979	2981	2983	rVB2	399	142	0.01%	0.001%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV120224\
 Data File : VV038391.D
 Acq On : 02 Dec 2024 16:14
 Operator : SY/MD
 Sample : VV1202MBL01
 Misc : 5.00g/5mL/100ul/5ML/MSVOA_V/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VBLK255

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\SFAMVLM120224WMA.M
 Title : VOC Analysis

77	10.657	2988	2991	2992	rBV2	559	253	0.01%	0.001%
78	10.824	3041	3043	3046	rVB2	738	339	0.01%	0.002%
79	10.866	3046	3056	3063	rBV9	2633	5001	0.22%	0.029%
80	10.915	3070	3071	3072	rBV9	429	150	0.01%	0.001%
81	10.943	3078	3080	3084	rBV3	580	395	0.02%	0.002%
82	10.963	3084	3086	3089	rBV	362	186	0.01%	0.001%
83	10.995	3093	3096	3101	rVB2	461	355	0.02%	0.002%
84	11.033	3101	3108	3113	rVB3	845	970	0.04%	0.006%
85	11.066	3113	3118	3121	rBV3	814	768	0.03%	0.004%
86	11.095	3125	3127	3130	rVB2	643	276	0.01%	0.002%
87	11.130	3130	3138	3142	rBV4	5591	8079	0.35%	0.047%
88	11.175	3142	3152	3181	rBV	959637	1557865	67.85%	9.018%
89	11.551	3257	3269	3295	rBV	1033407	1688952	73.56%	9.777%
90	12.181	3461	3465	3467	rBV2	1152	743	0.03%	0.004%
91	12.239	3478	3483	3485	rBV2	598	516	0.02%	0.003%
92	12.509	3563	3567	3571	rBV3	704	649	0.03%	0.004%
93	12.586	3583	3591	3606	rBV5	7263	14660	0.64%	0.085%
94	12.689	3617	3623	3627	rBV4	978	1030	0.04%	0.006%
95	12.747	3639	3641	3643	rVB	435	159	0.01%	0.001%
96	12.792	3652	3655	3658	rBV2	713	511	0.02%	0.003%
97	13.207	3775	3784	3794	rBV4	9582	18053	0.79%	0.105%
98	13.442	3846	3857	3879	rBV	23768	60332	2.63%	0.349%
99	13.937	4009	4011	4013	rBV3	679	259	0.01%	0.001%
100	14.696	4246	4247	4251	rBV3	907	643	0.03%	0.004%

Sum of corrected areas: 17274636

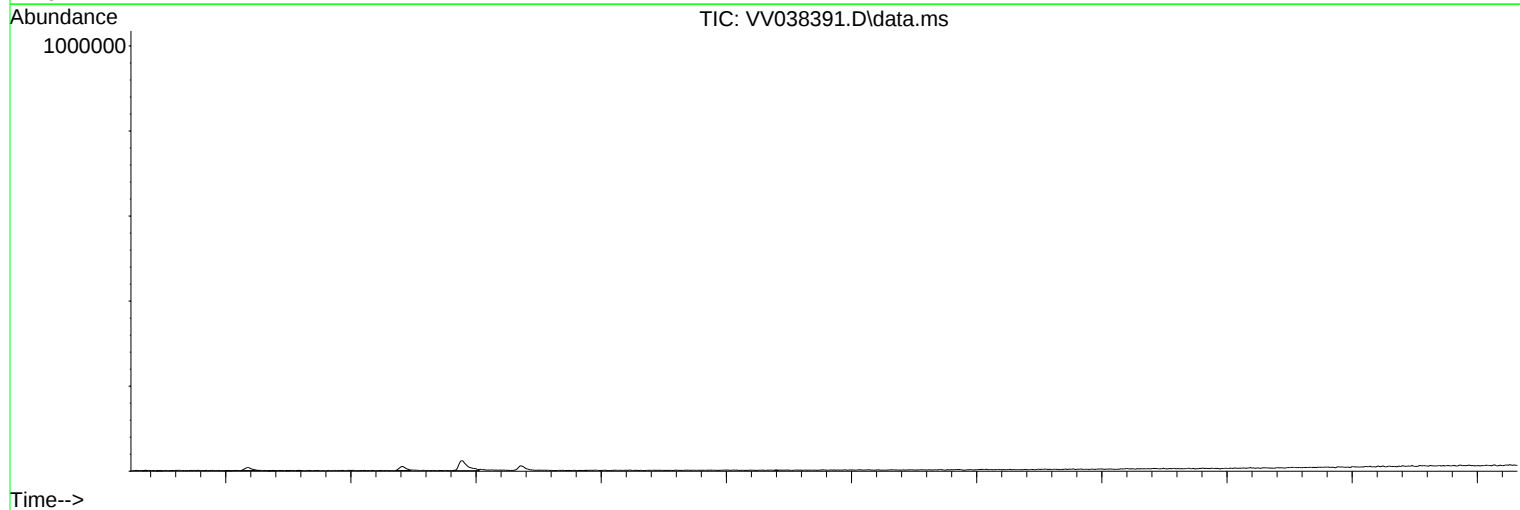
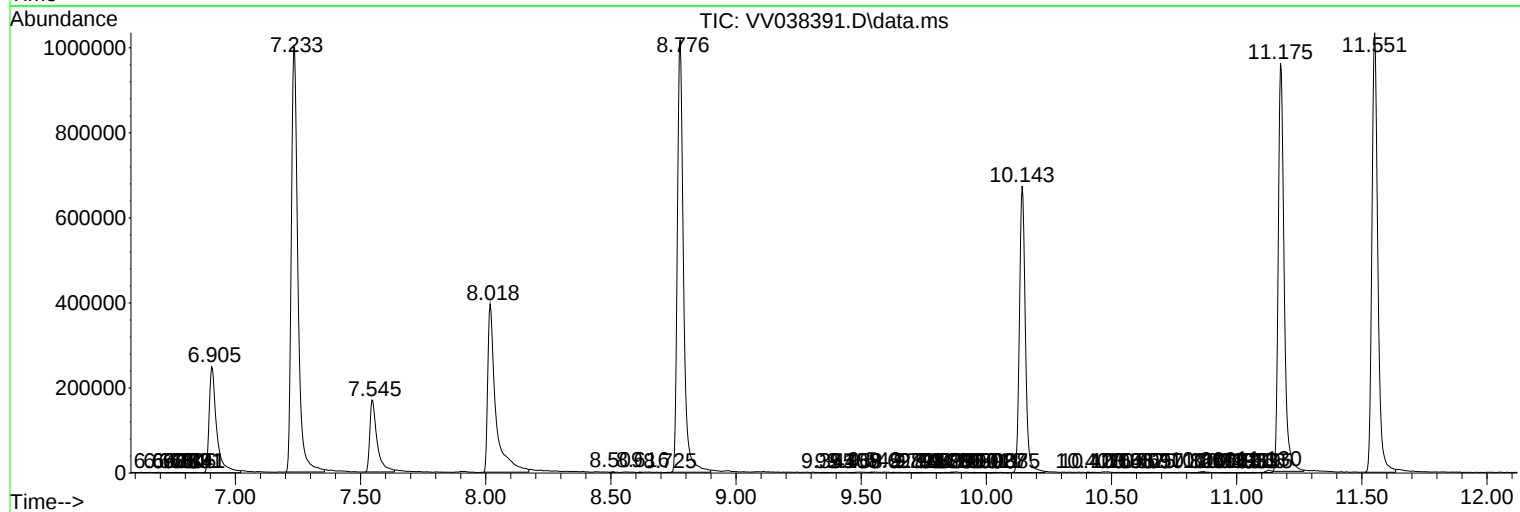
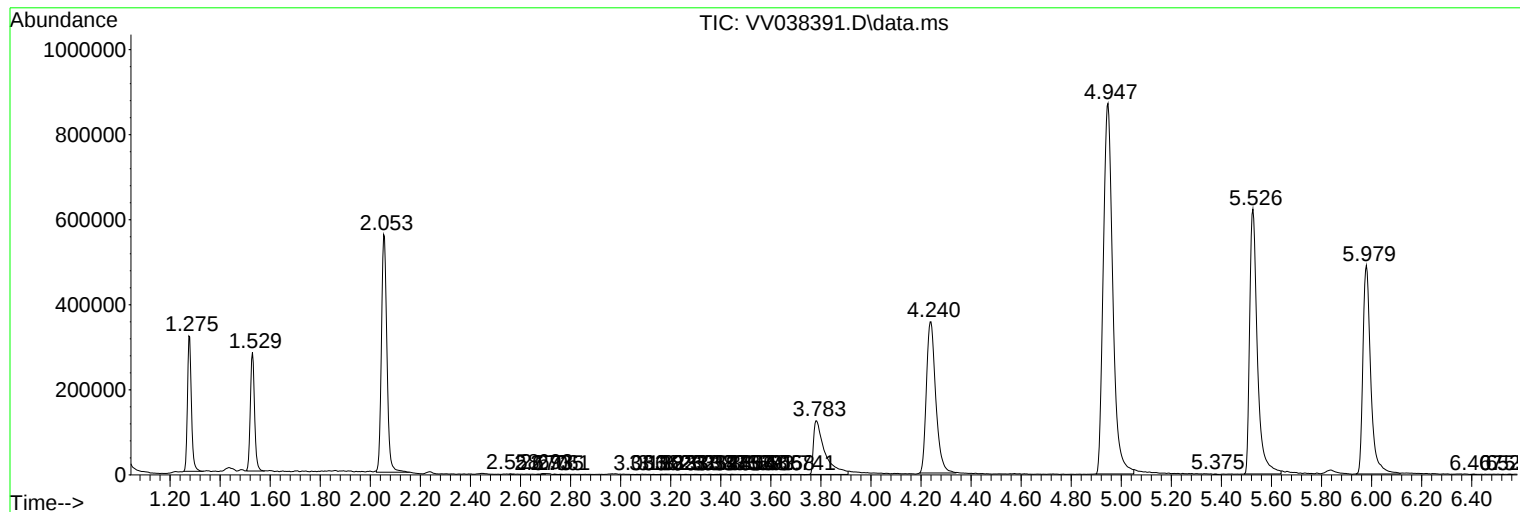
Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV120224\
Data File : VV038391.D
Acq On : 02 Dec 2024 16:14
Operator : SY/MD
Sample : VV1202MBL01
Misc : 5.00g/5mL/100ul/5ML/MSVOA_V/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VBLK255

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120224WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV120224\
Data File : VV038391.D
Acq On : 02 Dec 2024 16:14
Operator : SY/MD
Sample : VV1202MBL01
Misc : 5.00g/5mL/100ul/5ML/MSVOA_V/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VBLK255

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120224WMA.M
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\DATA\VV120224\
Data File : VV038391.D
Acq On : 02 Dec 2024 16:14
Operator : SY/MD
Sample : VV1202MBL01
Misc : 5.00g/5mL/100ul/5ML/MSVOA_V/MEOH
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VBLK255

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM120224WMA.M
Quant Title : VOC Analysis

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

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