

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051822\
 Data File : VU048617.D
 Acq On : 18 May 2022 16:32
 Operator : SY/MD
 Sample : N2843-13ME
 Misc : 7.01g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW4J3ME

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\SFAMULM051622WMA.M
 Title : VOC Analysis

Signal : TIC: VU048617.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	73	80	87	rBV	31049	40922	3.91%	0.549%
2	2.240	276	280	284	rBV2	317	316	0.03%	0.004%
3	2.324	303	306	307	rBV	317	173	0.02%	0.002%
4	2.533	358	371	383	rBV	101786	165223	15.79%	2.218%
5	2.729	427	432	436	rBV2	376	302	0.03%	0.004%
6	2.771	442	445	450	rBV2	342	230	0.02%	0.003%
7	2.884	478	480	485	rVB	270	174	0.02%	0.002%
8	2.912	486	489	493	rBV2	242	229	0.02%	0.003%
9	2.954	498	502	503	rBV2	499	338	0.03%	0.005%
10	3.028	518	525	527	rBV2	1687	2043	0.20%	0.027%
11	3.115	548	552	554	rBV	198	172	0.02%	0.002%
12	3.179	557	572	588	rBV	14052	33458	3.20%	0.449%
13	3.472	661	663	666	rBV	354	190	0.02%	0.003%
14	3.530	678	681	684	rBB2	286	204	0.02%	0.003%
15	3.591	697	700	706	rBV	215	255	0.02%	0.003%
16	3.671	722	725	728	rBB2	267	190	0.02%	0.003%
17	3.697	729	733	736	rBB	187	181	0.02%	0.002%
18	3.819	767	771	775	rBV	223	230	0.02%	0.003%
19	4.279	911	914	916	rVB	294	185	0.02%	0.002%
20	4.581	1006	1008	1010	rBV	310	191	0.02%	0.003%
21	4.629	1010	1023	1049	rBV2	87115	276658	26.45%	3.714%
22	4.874	1096	1099	1102	rBV2	334	268	0.03%	0.004%
23	4.980	1128	1132	1136	rBB2	228	171	0.02%	0.002%
24	5.060	1140	1157	1179	rBV	143519	338784	32.39%	4.548%
25	5.195	1196	1199	1203	rBV	488	345	0.03%	0.005%
26	5.266	1217	1221	1224	rBV	235	245	0.02%	0.003%
27	5.285	1224	1227	1232	rVB3	470	447	0.04%	0.006%
28	5.311	1232	1235	1236	rBV3	463	231	0.02%	0.003%
29	5.343	1236	1245	1247	rBV2	833	1051	0.10%	0.014%
30	5.424	1267	1270	1272	rBV2	360	194	0.02%	0.003%
31	5.568	1312	1315	1318	rBB2	281	177	0.02%	0.002%
32	5.716	1341	1361	1382	rBV2	256944	693268	66.27%	9.307%
33	5.973	1431	1441	1458	rVV4	6718	15034	1.44%	0.202%
34	6.102	1478	1481	1484	rVV	385	240	0.02%	0.003%
35	6.160	1496	1499	1501	rBV	448	294	0.03%	0.004%
36	6.247	1511	1526	1552	rBV	343378	691159	66.07%	9.279%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
 Title : VOC Analysis

37	6.414	1574	1578	1581	rBV	315	274	0.03%	0.004%
38	6.430	1581	1583	1585	rVB	329	168	0.02%	0.002%
39	6.523	1604	1612	1623	rVB4	5934	10299	0.98%	0.138%
40	6.597	1626	1635	1649	rBV3	3173	6887	0.66%	0.092%
41	6.690	1650	1664	1687	rVV	168062	345135	32.99%	4.633%
42	6.806	1695	1700	1705	rBB3	573	694	0.07%	0.009%
43	6.845	1709	1712	1715	rBV	164	172	0.02%	0.002%
44	6.925	1734	1737	1739	rBV	281	194	0.02%	0.003%
45	7.038	1770	1772	1775	rBV2	264	234	0.02%	0.003%
46	7.057	1775	1778	1781	rVB	419	290	0.03%	0.004%
47	7.189	1809	1819	1822	rBV3	5273	7352	0.70%	0.099%
48	7.308	1852	1856	1861	rVB3	393	362	0.03%	0.005%
49	7.420	1889	1891	1896	rBB	288	222	0.02%	0.003%
50	7.494	1907	1914	1918	rBB2	625	588	0.06%	0.008%
51	7.565	1921	1936	1956	rBV	91127	178489	17.06%	2.396%
52	7.655	1960	1964	1966	rBV	261	201	0.02%	0.003%
53	7.694	1972	1976	1979	rBV3	714	692	0.07%	0.009%
54	7.774	1997	2001	2002	rBV3	823	610	0.06%	0.008%
55	7.896	2025	2039	2055	rBV	263448	474448	45.35%	6.369%
56	8.041	2081	2084	2087	rVB2	423	254	0.02%	0.003%
57	8.182	2116	2128	2149	rBB2	64746	131637	12.58%	1.767%
58	8.282	2156	2159	2162	rBV	321	224	0.02%	0.003%
59	8.314	2167	2169	2173	rVB	366	214	0.02%	0.003%
60	8.536	2235	2238	2241	rBV	237	192	0.02%	0.003%
61	8.565	2245	2247	2250	rVB2	360	191	0.02%	0.003%
62	8.652	2256	2274	2303	rBV	284811	657767	62.88%	8.831%
63	8.838	2330	2332	2339	rBV	320	352	0.03%	0.005%
64	8.906	2351	2353	2355	rVB	511	173	0.02%	0.002%
65	8.922	2355	2358	2361	rBV	566	489	0.05%	0.007%
66	9.202	2437	2445	2449	rBV	206	384	0.04%	0.005%
67	9.231	2452	2454	2458	rVB	370	250	0.02%	0.003%
68	9.269	2462	2466	2467	rBV	338	230	0.02%	0.003%
69	9.420	2499	2513	2538	rBV	467958	891292	85.20%	11.966%
70	9.581	2560	2563	2566	rBV2	247	214	0.02%	0.003%
71	9.671	2587	2591	2594	rBV2	325	319	0.03%	0.004%
72	9.700	2597	2600	2609	rVB2	489	618	0.06%	0.008%
73	9.739	2610	2612	2614	rBV	300	169	0.02%	0.002%
74	9.986	2685	2689	2696	rBB	247	336	0.03%	0.005%
75	10.333	2794	2797	2799	rBV	217	175	0.02%	0.002%
76	10.655	2895	2897	2900	rBV	357	261	0.02%	0.004%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
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77	10.764	2918	2931	2952	rVB	367743	613087	58.61%	8.231%
78	10.899	2963	2973	2978	rVV4	1208	1723	0.16%	0.023%
79	11.118	3031	3041	3049	rVB5	4077	6257	0.60%	0.084%
80	11.150	3049	3051	3054	rBV	306	200	0.02%	0.003%
81	11.417	3128	3134	3143	rVB3	2185	2715	0.26%	0.036%
82	11.465	3143	3149	3153	rBV5	1166	1340	0.13%	0.018%
83	11.816	3245	3258	3276	rVV	668455	1046112	100.00%	14.044%
84	11.980	3306	3309	3311	rBV	832	655	0.06%	0.009%
85	12.095	3344	3345	3353	rVB2	358	303	0.03%	0.004%
86	12.198	3358	3377	3396	rBV	453296	732867	70.06%	9.839%
87	12.330	3411	3418	3428	rBV5	5075	7597	0.73%	0.102%
88	12.664	3519	3522	3530	rBV4	1620	1801	0.17%	0.024%
89	12.767	3551	3554	3560	rVV5	1007	1189	0.11%	0.016%
90	12.841	3571	3577	3583	rBV6	1125	1558	0.15%	0.021%
91	12.915	3596	3600	3601	rBV	860	556	0.05%	0.007%
92	13.054	3635	3643	3649	rBV7	1362	1882	0.18%	0.025%
93	13.134	3663	3668	3674	rVB4	1372	1545	0.15%	0.021%
94	13.237	3698	3700	3701	rBV4	662	255	0.02%	0.003%
95	13.433	3752	3761	3768	rBV5	9564	14744	1.41%	0.198%
96	13.587	3798	3809	3817	rBV6	7593	12553	1.20%	0.169%
97	13.713	3845	3848	3850	rBV3	693	531	0.05%	0.007%
98	13.812	3874	3879	3882	rBV3	922	776	0.07%	0.010%
99	13.838	3884	3887	3889	rBV2	952	685	0.07%	0.009%
100	14.452	4072	4078	4086	rVB3	15588	20996	2.01%	0.282%

Sum of corrected areas: 7448751

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.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\SFAMULM051622WMA.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
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