

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083122\
 Data File : VU050558.D
 Acq On : 31 Aug 2022 18:54
 Operator : SY/MD
 Sample : N4363-21ME
 Misc : 5.42g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVX5ME

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\SFAMULM083022WMA.M
 Title : VOC Analysis

Signal : TIC: VU050558.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.594	71	79	128	rBV	122830	248854	12.02%	1.642%
2	1.887	165	170	188	rBV	81185	134606	6.50%	0.888%
3	2.542	358	374	393	rBV	385894	628483	30.35%	4.148%
4	2.690	417	420	424	rBV3	339	282	0.01%	0.002%
5	2.758	438	441	442	rBV	354	229	0.01%	0.002%
6	2.793	450	452	459	rVB3	335	295	0.01%	0.002%
7	2.829	459	463	468	rBV2	232	329	0.02%	0.002%
8	2.864	471	474	477	rBV2	331	215	0.01%	0.001%
9	2.893	478	483	486	rBV2	196	169	0.01%	0.001%
10	2.912	486	489	492	rBV2	213	183	0.01%	0.001%
11	2.986	508	512	517	rBV3	346	367	0.02%	0.002%
12	3.124	553	555	558	rVB2	239	123	0.01%	0.001%
13	3.182	558	573	586	rBV2	5458	12269	0.59%	0.081%
14	3.353	624	626	628	rBV2	220	132	0.01%	0.001%
15	3.449	652	656	662	rBV	203	161	0.01%	0.001%
16	3.491	666	669	671	rBV	270	185	0.01%	0.001%
17	3.594	698	701	704	rBV2	200	170	0.01%	0.001%
18	3.684	722	729	734	rVB2	295	400	0.02%	0.003%
19	3.719	734	740	742	rBV2	275	296	0.01%	0.002%
20	3.774	755	757	760	rBV	257	187	0.01%	0.001%
21	3.915	799	801	805	rBV2	154	120	0.01%	0.001%
22	3.944	807	810	812	rBV	190	159	0.01%	0.001%
23	4.002	821	828	831	rBV2	190	288	0.01%	0.002%
24	4.067	842	848	851	rVB2	202	177	0.01%	0.001%
25	4.089	852	855	859	rBV	237	166	0.01%	0.001%
26	4.186	880	885	890	rBV2	202	235	0.01%	0.002%
27	4.266	905	910	911	rBV	202	188	0.01%	0.001%
28	4.292	915	918	922	rVB2	227	191	0.01%	0.001%
29	4.401	950	952	956	rBV2	156	122	0.01%	0.001%
30	4.558	994	1001	1004	rVB2	244	205	0.01%	0.001%
31	4.636	1008	1025	1081	rBV	158304	532460	25.71%	3.514%
32	5.060	1140	1157	1187	rBV	364884	809722	39.10%	5.344%
33	5.250	1211	1216	1219	rVB2	293	210	0.01%	0.001%
34	5.282	1219	1226	1228	rBV2	788	770	0.04%	0.005%
35	5.359	1244	1250	1252	rBV2	358	348	0.02%	0.002%
36	5.520	1299	1300	1306	rBV	159	119	0.01%	0.001%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM083022WMA.M
 Title : VOC Analysis

37	5.607	1318	1327	1328	rBV	198	158	0.01%	0.001%
38	5.719	1339	1362	1398	rBV2	809499	2070726	100.00%	13.667%
39	5.980	1430	1443	1453	rBV5	3879	8096	0.39%	0.053%
40	6.102	1478	1481	1483	rBV	350	278	0.01%	0.002%
41	6.247	1511	1526	1553	rBV	633825	1228382	59.32%	8.107%
42	6.410	1574	1577	1580	rBV2	338	278	0.01%	0.002%
43	6.526	1605	1613	1623	rVB6	2780	5086	0.25%	0.034%
44	6.600	1627	1636	1649	rBV3	1861	3507	0.17%	0.023%
45	6.690	1649	1664	1694	rVV	466670	939121	45.35%	6.198%
46	6.809	1694	1701	1708	rVB6	1259	1999	0.10%	0.013%
47	6.841	1709	1711	1713	rBV2	370	190	0.01%	0.001%
48	6.899	1728	1729	1734	rVV	186	120	0.01%	0.001%
49	6.922	1734	1736	1743	rVB	216	174	0.01%	0.001%
50	7.015	1761	1765	1769	rBV2	209	173	0.01%	0.001%
51	7.192	1814	1820	1822	rBV3	1209	1117	0.05%	0.007%
52	7.359	1869	1872	1874	rBV2	205	164	0.01%	0.001%
53	7.433	1893	1895	1899	rVB2	221	141	0.01%	0.001%
54	7.484	1908	1911	1917	rVB	288	268	0.01%	0.002%
55	7.565	1923	1936	1960	rBV	221242	409138	19.76%	2.700%
56	7.687	1970	1974	1975	rBV2	369	288	0.01%	0.002%
57	7.809	2006	2012	2016	rBV3	282	273	0.01%	0.002%
58	7.835	2017	2020	2022	rBV2	204	144	0.01%	0.001%
59	7.896	2022	2039	2062	rBV	929801	1627789	78.61%	10.744%
60	8.182	2115	2128	2153	rBV	146976	272632	13.17%	1.799%
61	8.320	2170	2171	2174	rVB2	340	126	0.01%	0.001%
62	8.552	2232	2243	2256	rBV3	17879	28611	1.38%	0.189%
63	8.652	2259	2274	2308	rBV2	513906	1165147	56.27%	7.690%
64	8.935	2360	2362	2366	rBV2	273	169	0.01%	0.001%
65	8.983	2375	2377	2381	rVB2	184	134	0.01%	0.001%
66	9.005	2381	2384	2386	rBV	208	170	0.01%	0.001%
67	9.124	2417	2421	2423	rBV2	275	239	0.01%	0.002%
68	9.301	2473	2476	2480	rBV2	284	252	0.01%	0.002%
69	9.420	2499	2513	2548	rBV	840749	1462722	70.64%	9.654%
70	9.610	2566	2572	2574	rBV3	422	392	0.02%	0.003%
71	9.697	2596	2599	2602	rBV	298	201	0.01%	0.001%
72	9.947	2674	2677	2681	rBV3	394	330	0.02%	0.002%
73	10.047	2704	2708	2710	rBV2	192	140	0.01%	0.001%
74	10.205	2754	2757	2759	rBV2	214	166	0.01%	0.001%
75	10.295	2783	2785	2788	rBV2	192	138	0.01%	0.001%
76	10.600	2878	2880	2883	rBV	217	119	0.01%	0.001%

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM083022WMA.M
 Title : VOC Analysis

77	10.619	2884	2886	2896	rVB2	255	313	0.02%	0.002%
78	10.661	2896	2899	2907	rBV	135	132	0.01%	0.001%
79	10.700	2908	2911	2914	rVB	215	122	0.01%	0.001%
80	10.761	2914	2930	2953	rBV	685985	1114750	53.83%	7.357%
81	10.915	2973	2978	2982	rBV2	352	301	0.01%	0.002%
82	10.938	2982	2985	2989	rBV	222	191	0.01%	0.001%
83	11.024	3010	3012	3015	rVB2	316	163	0.01%	0.001%
84	11.115	3036	3040	3042	rBV2	662	413	0.02%	0.003%
85	11.256	3079	3084	3089	rBV2	321	458	0.02%	0.003%
86	11.307	3096	3100	3103	rBV	179	159	0.01%	0.001%
87	11.452	3141	3145	3146	rBV2	190	127	0.01%	0.001%
88	11.658	3207	3209	3212	rBV	174	125	0.01%	0.001%
89	11.815	3243	3258	3281	rBV	733174	1140476	55.08%	7.527%
90	12.195	3363	3376	3403	rBV	820934	1288495	62.22%	8.504%
91	12.381	3431	3434	3436	rBV2	471	356	0.02%	0.002%
92	12.587	3495	3498	3503	rBV	198	156	0.01%	0.001%
93	12.619	3504	3508	3511	rVB2	354	300	0.01%	0.002%
94	12.648	3514	3517	3519	rBV2	294	149	0.01%	0.001%
95	13.002	3623	3627	3631	rVB2	265	214	0.01%	0.001%
96	13.102	3655	3658	3661	rBV2	370	250	0.01%	0.002%
97	13.127	3664	3666	3670	rVB2	333	193	0.01%	0.001%
98	13.648	3826	3828	3830	rBV	328	191	0.01%	0.001%
99	13.825	3880	3883	3885	rBV	369	231	0.01%	0.002%
100	13.921	3909	3913	3915	rBV	341	285	0.01%	0.002%

Sum of corrected areas: 15151263

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Instrument :
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DBVX5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM083022WMA.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 :
DBVX5ME

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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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