

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU113021\
 Data File : VU046030.D
 Acq On : 30 Nov 2021 16:57
 Operator : SY/MD
 Sample : M4833-24ME
 Misc : 5.50g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ESQP7ME

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\SFAMULM112921WMA.M
 Title : VOC Analysis

Signal : TIC: VU046030.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.600	74	81	100	rVB	77274	104920	13.89%	1.767%
2	1.919	171	180	201	rBV	51174	87833	11.63%	1.479%
3	2.552	368	377	391	rVB	120953	192172	25.44%	3.237%
4	3.182	559	573	591	rBV2	9280	23218	3.07%	0.391%
5	3.346	619	624	632	rVB5	1370	2124	0.28%	0.036%
6	3.478	663	665	668	rBV	133	115	0.02%	0.002%
7	3.520	676	678	681	rBB	167	111	0.01%	0.002%
8	3.552	682	688	691	rBB	178	193	0.03%	0.003%
9	3.697	729	733	737	rBB	129	160	0.02%	0.003%
10	3.867	773	786	798	rBV	2719	5627	0.74%	0.095%
11	4.668	1016	1035	1083	rBV	49982	222826	29.50%	3.753%
12	5.066	1144	1159	1187	rVB	119790	294314	38.97%	4.957%
13	5.259	1217	1219	1223	rBV	156	148	0.02%	0.002%
14	5.314	1223	1236	1250	rVB4	4983	10860	1.44%	0.183%
15	5.529	1300	1303	1306	rBV	124	133	0.02%	0.002%
16	5.726	1343	1364	1385	rBV2	294269	755321	100.00%	12.722%
17	5.989	1435	1446	1458	rBV6	3325	8924	1.18%	0.150%
18	6.253	1513	1528	1555	rVV	224217	456488	60.44%	7.689%
19	6.542	1606	1618	1633	rBV2	37370	74081	9.81%	1.248%
20	6.693	1652	1665	1690	rVB	164497	337209	44.64%	5.680%
21	6.793	1693	1696	1698	rBV	151	122	0.02%	0.002%
22	6.812	1698	1702	1705	rVB2	222	163	0.02%	0.003%
23	7.192	1811	1820	1824	rBV4	1204	1574	0.21%	0.027%
24	7.230	1830	1832	1834	rVB	272	132	0.02%	0.002%
25	7.571	1923	1938	1963	rBV	85436	168869	22.36%	2.844%
26	7.690	1970	1975	1979	rBV	565	580	0.08%	0.010%
27	7.709	1979	1981	1988	rVB2	347	280	0.04%	0.005%
28	7.748	1989	1993	1996	rBV	165	116	0.02%	0.002%
29	7.799	1997	2009	2016	rBV5	2336	4453	0.59%	0.075%
30	7.902	2026	2041	2061	rBV	305569	593089	78.52%	9.990%
31	8.185	2118	2129	2155	rVV2	48281	113690	15.05%	1.915%
32	8.362	2180	2184	2188	rBB	179	188	0.02%	0.003%
33	8.452	2208	2212	2215	rBV	159	191	0.03%	0.003%
34	8.475	2217	2219	2224	rVV2	250	234	0.03%	0.004%
35	8.561	2238	2246	2251	rBV4	1294	1869	0.25%	0.031%
36	8.687	2262	2285	2319	rBV2	117037	391324	51.81%	6.591%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

37	8.803	2319	2321	2325	rBV	245	153	0.02%	0.003%
38	8.880	2340	2345	2346	rBV	141	120	0.02%	0.002%
39	9.066	2400	2403	2406	rBB	137	115	0.02%	0.002%
40	9.124	2418	2421	2423	rBV	131	113	0.01%	0.002%
41	9.169	2431	2435	2439	rBV	135	182	0.02%	0.003%
42	9.256	2458	2462	2465	rBB	150	152	0.02%	0.003%
43	9.324	2480	2483	2484	rBV	153	106	0.01%	0.002%
44	9.372	2494	2498	2499	rBV	127	112	0.01%	0.002%
45	9.430	2501	2516	2537	rVV	242238	568504	75.27%	9.576%
46	9.539	2545	2550	2552	rBB	146	149	0.02%	0.003%
47	9.661	2585	2588	2590	rBV	259	127	0.02%	0.002%
48	9.703	2593	2601	2610	rVV	1287	2386	0.32%	0.040%
49	9.745	2610	2614	2619	rVB2	540	504	0.07%	0.008%
50	9.889	2655	2659	2661	rBV	143	153	0.02%	0.003%
51	10.066	2711	2714	2718	rBB	149	152	0.02%	0.003%
52	10.111	2721	2728	2730	rBV	615	745	0.10%	0.013%
53	10.240	2765	2768	2771	rVB2	302	223	0.03%	0.004%
54	10.262	2772	2775	2779	rBV	124	161	0.02%	0.003%
55	10.487	2841	2845	2847	rBV2	387	350	0.05%	0.006%
56	10.674	2895	2903	2911	rBV2	2947	4163	0.55%	0.070%
57	10.777	2920	2935	2949	rBV	224260	383578	50.78%	6.461%
58	10.870	2956	2964	2967	rBV4	439	578	0.08%	0.010%
59	11.005	2998	3006	3009	rBV	811	877	0.12%	0.015%
60	11.095	3029	3034	3035	rBV	462	397	0.05%	0.007%
61	11.211	3067	3070	3074	rBV2	177	133	0.02%	0.002%
62	11.349	3110	3113	3115	rBV	153	132	0.02%	0.002%
63	11.423	3130	3136	3139	rBV3	292	293	0.04%	0.005%
64	11.465	3141	3149	3151	rBV2	2482	3010	0.40%	0.051%
65	11.549	3172	3175	3178	rBV	178	170	0.02%	0.003%
66	11.568	3179	3181	3183	rBV	204	119	0.02%	0.002%
67	11.700	3215	3222	3228	rBV4	1432	1854	0.25%	0.031%
68	11.754	3234	3239	3247	rVB2	811	868	0.11%	0.015%
69	11.822	3247	3260	3280	rBV	350131	546698	72.38%	9.208%
70	11.947	3293	3299	3302	rBV3	979	1157	0.15%	0.019%
71	12.102	3345	3347	3350	rBV2	319	238	0.03%	0.004%
72	12.204	3366	3379	3393	rVB	323233	524681	69.46%	8.838%
73	12.275	3393	3401	3403	rBV2	281	310	0.04%	0.005%
74	12.288	3403	3405	3411	rVB	222	117	0.02%	0.002%
75	12.333	3411	3419	3426	rBV2	4844	6730	0.89%	0.113%
76	12.384	3431	3435	3436	rBV2	623	308	0.04%	0.005%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
 Title : VOC Analysis

77	12.638	3509	3514	3519	rBV2	409	404	0.05%	0.007%
78	12.674	3522	3525	3526	rBV2	262	129	0.02%	0.002%
79	12.712	3534	3537	3539	rBV2	373	245	0.03%	0.004%
80	12.947	3606	3610	3613	rBV2	207	199	0.03%	0.003%
81	13.224	3691	3696	3706	rBV4	1032	1269	0.17%	0.021%
82	13.359	3736	3738	3739	rBV4	251	105	0.01%	0.002%
83	13.433	3754	3761	3777	rVB4	4781	7321	0.97%	0.123%
84	13.558	3797	3800	3804	rBV2	218	220	0.03%	0.004%
85	13.587	3804	3809	3816	rVB4	1116	1434	0.19%	0.024%
86	13.847	3882	3890	3896	rBV6	1500	1852	0.25%	0.031%
87	14.044	3948	3951	3955	rBV3	434	267	0.04%	0.004%
88	14.095	3960	3967	3976	rVB	2921	4133	0.55%	0.070%
89	14.195	3989	3998	4004	rVB4	1356	2040	0.27%	0.034%
90	14.333	4035	4041	4050	rVB2	1563	2165	0.29%	0.036%
91	14.404	4061	4063	4067	rVB	333	161	0.02%	0.003%
92	14.452	4071	4078	4085	rVB4	4243	5834	0.77%	0.098%
93	14.587	4118	4120	4122	rBV	336	152	0.02%	0.003%
94	14.944	4227	4231	4232	rBV	651	476	0.06%	0.008%
95	15.018	4251	4254	4259	rVB2	578	349	0.05%	0.006%
96	15.053	4262	4265	4268	rBV	568	504	0.07%	0.008%
97	15.150	4289	4295	4302	rBV4	787	790	0.10%	0.013%
98	15.208	4308	4313	4315	rBV4	1307	1254	0.17%	0.021%
99	15.497	4401	4403	4407	rBV4	577	466	0.06%	0.008%
100	15.603	4434	4436	4439	rBV3	819	575	0.08%	0.010%

Sum of corrected areas: 5936913

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ESQP7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.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 :
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ClientSampleId :
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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	--Internal Standard--			
					#	RT	Resp	Conc