LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022522\
Data File : VU047269.D
Acq On : 25 Feb 2022 13:46
Operator : SY/MD
Sample : N1631-15ME
Misc : 5.88g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : DBRJ1ME

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\SFAMULM021022WMA.M
Title : VOC Analysis

Signal : TIC: VU047269.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.520	51	56	69	rVB2	5469	8083	0.72%	0.081%
2	1.601	74	81	87	rBV	53358	74177	6.58%	0.746%
3	1.916	173	179	185	rBV	25033	36475	3.23%	0.367%
4	2.543	365	374	424	rVB	272316	551379	48.89%	5.545%
5	2.993	511	514	515	rBV2	317	189	0.02%	0.002%
6	3.112	549	551	553	rVB3	430	146	0.01%	0.001%
7	3.150	559	563	564	rVV2	659	432	0.04%	0.004%
8	3.173	564	570	585	rVB5	2547	5451	0.48%	0.055%
9	3.231	585	588	589	rBV2	282	106	0.01%	0.001%
10	3.282	600	604	605	rBV	308	205	0.02%	0.002%
11	3.363	627	629	634	rBV2	316	202	0.02%	0.002%
12	3.385	634	636	637	rVV	314	106	0.01%	0.001%
13	3.511	672	675	677	rBV	166	122	0.01%	0.001%
14	3.556	686	689	691	rVV2	220	150	0.01%	0.002%
15	3.575	691	695	698	rVV3	383	310	0.03%	0.003%
16	3.633	709	713	716	rBV2	227	193	0.02%	0.002%
17	3.697	731	733	738	rVB2	258	131	0.01%	0.001%
18	3.816	765	770	771	rBV2	210	182	0.02%	0.002%
19	3.922	800	803	807	rBV	177	137	0.01%	0.001%
20	4.054	841	844	852	rVB3	231	297	0.03%	0.003%
21	4.099	852	858	865	rBV2	232	284	0.03%	0.003%
22	4.131	865	868	870	rBV	140	106	0.01%	0.001%
23	4.186	882	885	888	rBV2	193	148	0.01%	0.001%
24	4.205	889	891	895	rVB2	156	105	0.01%	0.001%
25	4.237	895	901	904	rBV3	177	212	0.02%	0.002%
26	4.301	916	921	924	rBV2	152	129	0.01%	0.001%
27	4.440	959	964	967	rVB3	167	161	0.01%	0.002%
28	4.498	976	982	985	rBV3	224	240	0.02%	0.002%
29	4.517	985	988	994	rVB2	138	138	0.01%	0.001%
30	4.578	1001	1007	1009	rBV3	137	143	0.01%	0.001%
31	4.655	1014	1031	1048	rBV	58970	215571	19.11%	2.168%
32	5.067	1143	1159	1195	rVB	174176	441718	39.16%	4.442%
33	5.227	1206	1209	1213	rBV2	206	175	0.02%	0.002%
34	5.256	1213	1218	1221	rBV3	134	126	0.01%	0.001%
35	5.295	1223	1230	1236	rBV5	507	692	0.06%	0.007%
36	5.346	1238	1246	1250	rBV2	681	887	0.08%	0.009%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022522\
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Operator : SY/MD
Sample : N1631-15ME
Misc : 5.88g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBRJ1ME

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\SFAMULM021022WMA.M
Title : VOC Analysis

37	5.523	1299	1301	1307	rVB2	218	169	0.01%	0.002%
38	5.562	1310	1313	1319	rBV2	218	231	0.02%	0.002%
39	5.636	1332	1336	1338	rBV2	179	130	0.01%	0.001%
40	5.723	1341	1363	1396	rVV2	446688	1127854	100.00%	11.343%
41	5.877	1409	1411	1415	rVB2	227	112	0.01%	0.001%
42	5.903	1415	1419	1420	rBV	222	149	0.01%	0.001%
43	5.983	1431	1444	1457	rBV3	9350	25526	2.26%	0.257%
44	6.105	1479	1482	1484	rBV2	291	188	0.02%	0.002%
45	6.125	1484	1488	1490	rVB2	256	210	0.02%	0.002%
46	6.147	1492	1495	1497	rBV	229	159	0.01%	0.002%
47	6.176	1497	1504	1511	rBV3	655	867	0.08%	0.009%
48	6.250	1513	1527	1557	rVB	230376	501108	44.43%	5.040%
49	6.356	1557	1560	1565	rVB4	398	295	0.03%	0.003%
50	6.427	1579	1582	1586	rVB2	195	150	0.01%	0.002%
51	6.449	1586	1589	1594	rBV2	166	130	0.01%	0.001%
52	6.481	1594	1599	1602	rBV2	304	260	0.02%	0.003%
53	6.533	1604	1615	1625	rBV6	2715	5763	0.51%	0.058%
54	6.607	1629	1638	1646	rBV6	3700	7034	0.62%	0.071%
55	6.694	1651	1665	1696	rVB	222991	499486	44.29%	5.023%
56	6.874	1718	1721	1726	rBV2	221	134	0.01%	0.001%
57	6.935	1733	1740	1743	rBV2	428	538	0.05%	0.005%
58	7.015	1762	1765	1766	rBV2	195	126	0.01%	0.001%
59	7.192	1811	1820	1822	rBV3	1005	1452	0.13%	0.015%
60	7.231	1823	1832	1833	rBV6	3171	3646	0.32%	0.037%
61	7.372	1874	1876	1879	rVB2	237	113	0.01%	0.001%
62	7.414	1882	1889	1893	rBV3	196	229	0.02%	0.002%
63	7.507	1913	1918	1922	rVB2	188	163	0.01%	0.002%
64	7.568	1922	1937	1965	rBV	121224	272972	24.20%	2.745%
65	7.684	1969	1973	1975	rBV3	623	560	0.05%	0.006%
66	7.800	1999	2009	2014	rBV5	868	1435	0.13%	0.014%
67	7.903	2024	2041	2059	rBV	494290	993815	88.12%	9.995%
68	8.131	2108	2112	2114	rBV3	196	177	0.02%	0.002%
69	8.186	2116	2129	2156	rBV	69621	187976	16.67%	1.891%
70	8.330	2172	2174	2176	rBV	220	99	0.01%	0.001%
71	8.475	2205	2219	2239	rBV2	10904	23071	2.05%	0.232%
72	8.687	2260	2285	2313	rBV	228463	697485	61.84%	7.015%
73	8.796	2316	2319	2327	rBV4	791	1138	0.10%	0.011%
74	8.967	2369	2372	2378	rVB3	176	184	0.02%	0.002%
75	9.041	2393	2395	2398	rBV2	156	102	0.01%	0.001%
76	9.276	2465	2468	2473	rBV2	177	136	0.01%	0.001%

LSC Area Percent Report

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Sample : N1631-15ME
Misc : 5.88g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBRJ1ME

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\SFAMULM021022WMA.M
Title : VOC Analysis

77	9.308	2473	2478	2480	rBV2	165	155	0.01%	0.002%
78	9.343	2484	2489	2491	rBV2	215	184	0.02%	0.002%
79	9.359	2491	2494	2498	rVB3	316	210	0.02%	0.002%
80	9.427	2501	2515	2538	rBV	284974	670321	59.43%	6.742%
81	10.623	2884	2887	2891	rBV3	687	641	0.06%	0.006%
82	10.674	2894	2903	2913	rVB	9504	15235	1.35%	0.153%
83	10.774	2921	2934	2950	rBV	367088	606974	53.82%	6.104%
84	10.899	2966	2973	2989	rVB	14094	25064	2.22%	0.252%
85	11.118	3033	3041	3049	rBV3	6867	11178	0.99%	0.112%
86	11.314	3098	3102	3108	rBV7	884	1009	0.09%	0.010%
87	11.459	3141	3147	3169	rVB3	6963	13406	1.19%	0.135%
88	11.581	3179	3185	3197	rVB4	2064	3460	0.31%	0.035%
89	11.700	3214	3222	3233	rBV3	5354	8426	0.75%	0.085%
90	11.822	3247	3260	3272	rBV	472033	744574	66.02%	7.488%
91	12.201	3360	3378	3393	rBV	565759	919060	81.49%	9.243%
92	12.333	3413	3419	3427	rVB6	3503	5281	0.47%	0.053%
93	12.385	3431	3435	3436	rBV2	1363	883	0.08%	0.009%
94	12.526	3474	3479	3480	rBV2	1416	1078	0.10%	0.011%
95	12.777	3550	3557	3568	rVB2	6753	9619	0.85%	0.097%
96	13.774	3865	3867	3868	rBV2	596	288	0.03%	0.003%
97	14.118	3970	3974	3976	rBV5	1163	956	0.08%	0.010%
98	14.169	3988	3990	3992	rBV2	753	458	0.04%	0.005%
99	16.359	4660	4671	4693	rBV	730949	1097534	97.31%	11.038%
100	16.889	4828	4836	4849	rBV	73978	112420	9.97%	1.131%

Sum of corrected areas: 9943094

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022522\
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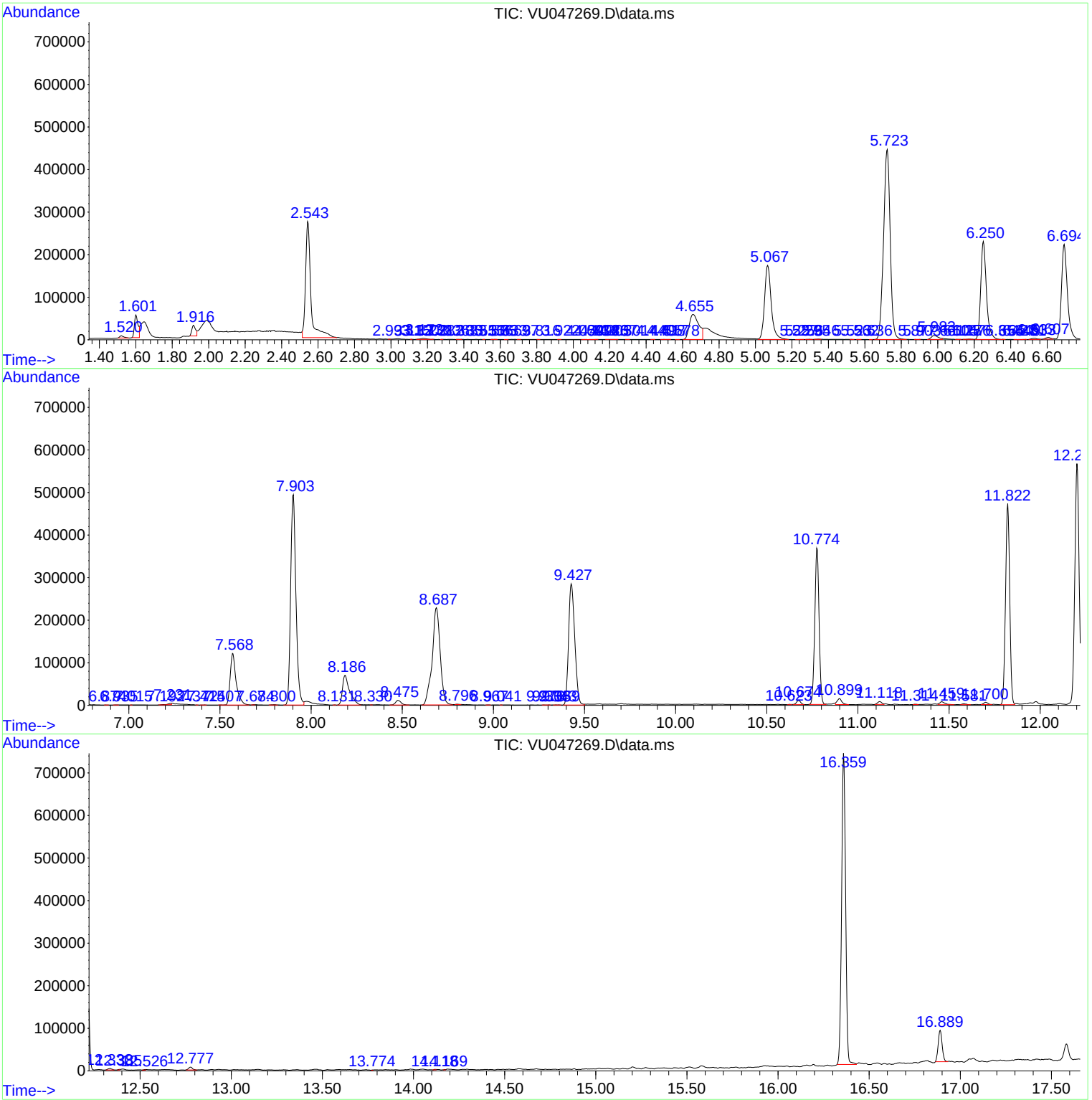
Operator : SY/MD
Sample : N1631-15ME
Misc : 5.88g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBRJ1ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021022WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022522\
Data File : VU047269.D
Acq On : 25 Feb 2022 13:46
Operator : SY/MD
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBRJ1ME

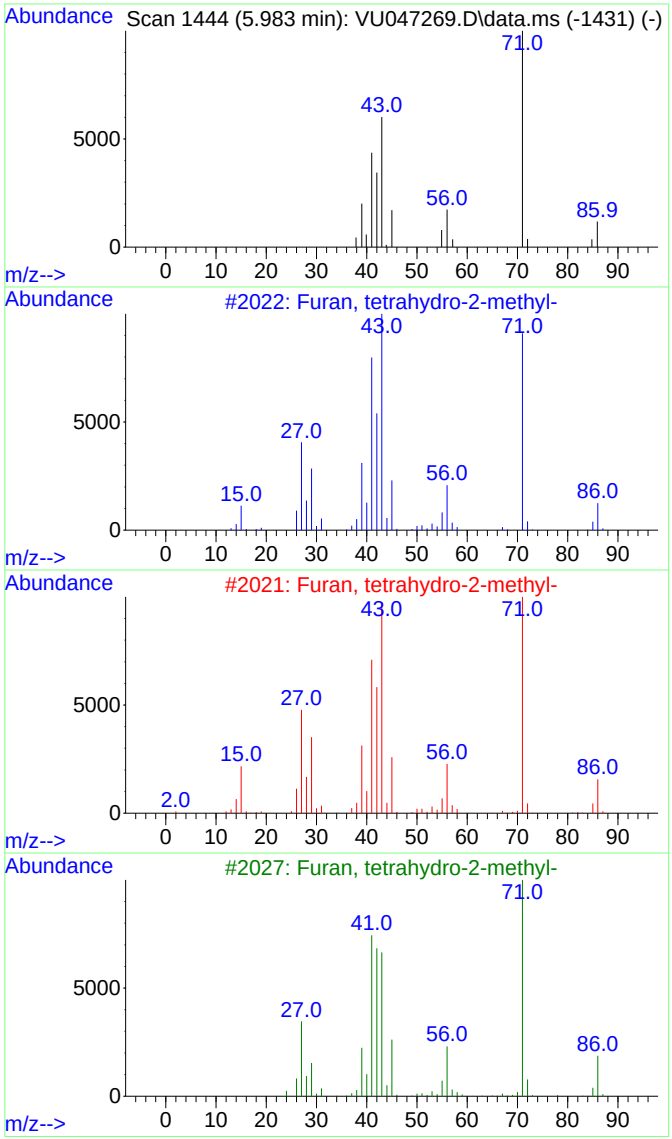
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021022WMA.M
Quant Title : VOC Analysis

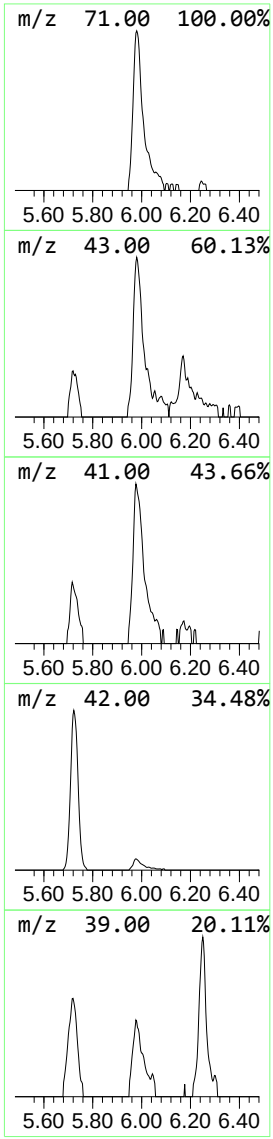
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Furan, tetrahydro-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.983	2.55 ug/L	25526	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	91
2	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	76
3	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	50
4	3-Penten-2-ol	86	C5H10O	001569-50-2	45
5	2-Butene, 1-methoxy-, (E)-	86	C5H10O	010034-14-7	35





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022522\
Data File : VU047269.D
Acq On : 25 Feb 2022 13:46
Operator : SY/MD
Sample : N1631-15ME
Misc : 5.88g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBRJ1ME

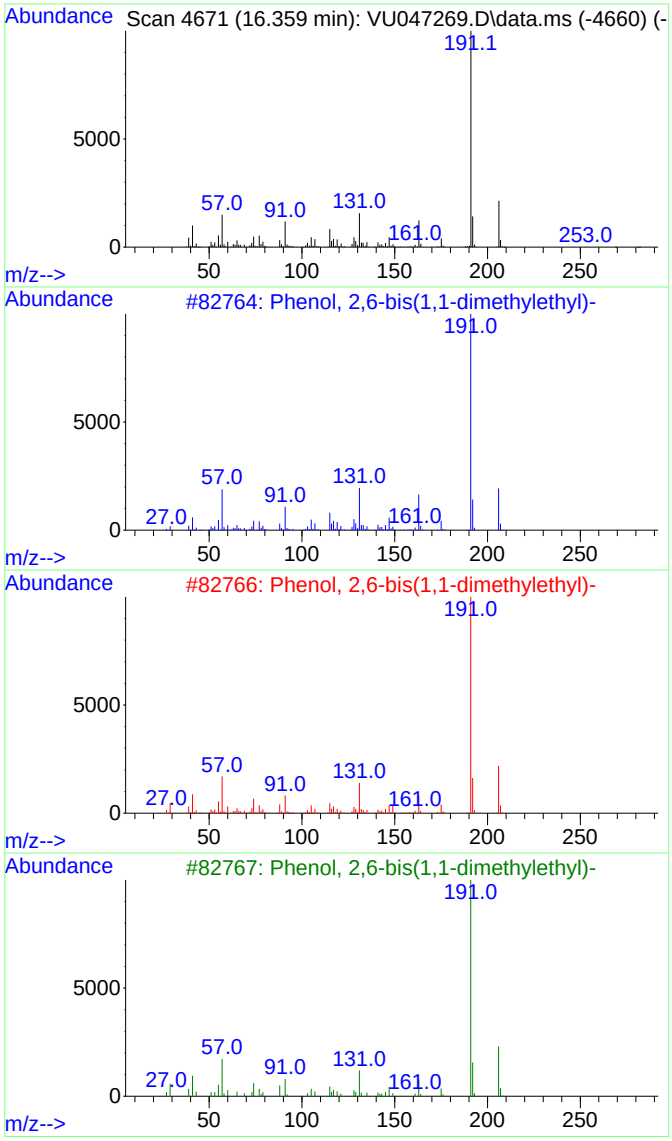
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021022WMA.M
Quant Title : VOC Analysis

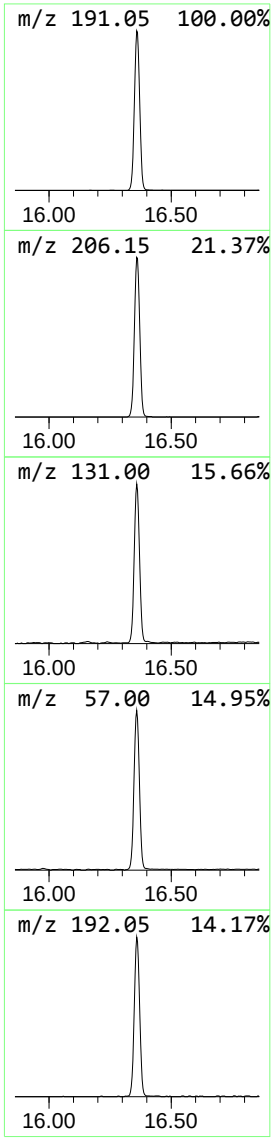
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.359	73.70 ug/L	1097530	1,4-Dichlorobenzene-d4	11.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	98
2	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	97
3	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	95
4	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	93
5	2,4-Di-tert-butylphenol	206	C14H22O	000096-76-4	93





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Operator : SY/MD
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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBRJ1ME

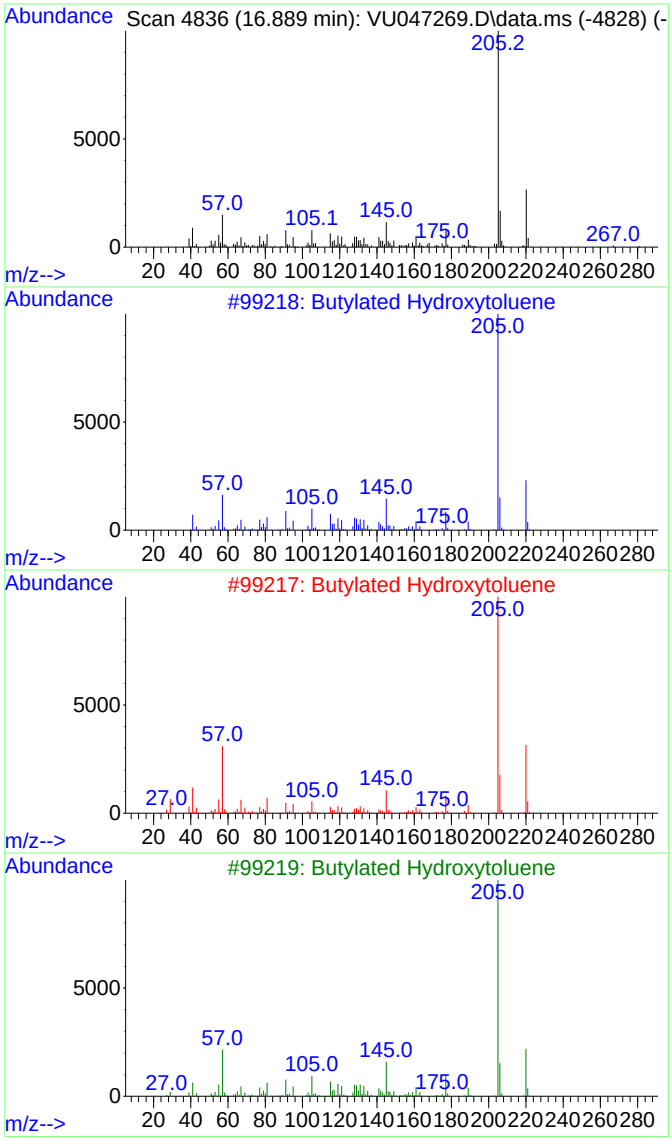
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021022WMA.M
Quant Title : VOC Analysis

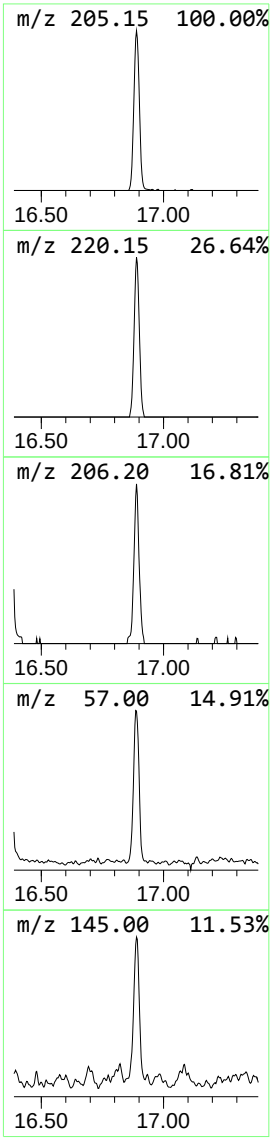
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Butylated Hydroxytoluene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.889	7.55 ug/L	112420	1,4-Dichlorobenzene-d4	11.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	97
2	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	97
3	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	96
4	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	96
5	Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU022522\
Data File : VU047269.D
Acq On : 25 Feb 2022 13:46
Operator : SY/MD
Sample : N1631-15ME
Misc : 5.88g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBRJ1ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM021022WMA.M
Quant Title : VOC Analysis

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Furan, tetrahyd...	5.983	2.5	ug/L	25526	1	6.250	501108	50.0
Phenol, 2,6-bis...	16.359	73.7	ug/L	1097530	3	11.822	744574	50.0
Butylated Hydro...	16.889	7.5	ug/L	112420	3	11.822	744574	50.0