LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072924\
Data File : VX042695.D
Acq On : 29 Jul 2024 17:00
Operator : JC/MD
Sample : P3344-03ME
Misc : 4.76g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BHB19ME

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_X\Method\SFAMXLM072624WMA.M
Title : VOC Analysis

Signal : TIC: VX042695.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.167	11	13	15	rBV	689	430	0.11%	0.013%
2	1.258	25	28	36	rVB2	8108	9881	2.49%	0.302%
3	1.374	43	47	49	rBV2	27468	38348	9.67%	1.170%
4	1.557	73	77	78	rBV3	1185	1505	0.38%	0.046%
5	1.630	86	89	94	rBV2	12432	24389	6.15%	0.744%
6	2.276	190	195	211	rBV	53820	102683	25.89%	3.133%
7	2.563	240	242	245	rBV2	313	315	0.08%	0.010%
8	2.605	248	249	251	rBV	387	365	0.09%	0.011%
9	2.721	263	268	274	rVV2	4167	8021	2.02%	0.245%
10	2.941	296	304	311	rBV3	1673	4129	1.04%	0.126%
11	3.081	320	327	334	rBV	11610	21810	5.50%	0.666%
12	3.288	359	361	364	rVV2	218	275	0.07%	0.008%
13	3.501	393	396	398	rBV	240	314	0.08%	0.010%
14	3.776	438	441	443	rBV	204	282	0.07%	0.009%
15	4.026	476	482	484	rBV2	180	380	0.10%	0.012%
16	4.306	526	528	530	rBV2	306	274	0.07%	0.008%
17	4.392	538	542	548	rBV2	280	503	0.13%	0.015%
18	4.489	550	558	574	rBV	24582	85810	21.64%	2.619%
19	5.056	639	651	669	rBV	51307	160306	40.42%	4.892%
20	5.385	703	705	709	rBV3	356	563	0.14%	0.017%
21	5.538	728	730	732	rVV2	375	318	0.08%	0.010%
22	5.562	732	734	736	rVV	338	304	0.08%	0.009%
23	5.605	739	741	745	rVB	217	263	0.07%	0.008%
24	5.660	745	750	751	rBV2	252	383	0.10%	0.012%
25	5.964	789	800	813	rBV3	140089	396596	100.00%	12.102%
26	6.153	829	831	835	rVB	544	413	0.10%	0.013%
27	6.190	835	837	840	rBV2	282	259	0.07%	0.008%
28	6.281	849	852	854	rBV2	235	289	0.07%	0.009%
29	6.379	865	868	870	rBV2	263	337	0.08%	0.010%
30	6.757	921	930	943	rBV2	129854	315415	79.53%	9.625%
31	6.970	964	965	967	rBV	415	249	0.06%	0.008%
32	7.129	984	991	996	rVB5	1889	3988	1.01%	0.122%
33	7.306	1012	1020	1030	rBV	78389	177202	44.68%	5.407%
34	7.860	1107	1111	1113	rVB2	235	300	0.08%	0.009%
35	7.891	1113	1116	1118	rBV	224	267	0.07%	0.008%
36	7.964	1126	1128	1129	rBV	486	324	0.08%	0.010%

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Misc : 4.76g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BHB19ME

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Title : VOC Analysis

37	8.324	1181	1187	1197	rBV	41710	72365	18.25%	2.208%
38	8.507	1214	1217	1220	rBV2	394	542	0.14%	0.017%
39	8.543	1221	1223	1225	rVB2	536	441	0.11%	0.013%
40	8.592	1228	1231	1234	rBV	255	270	0.07%	0.008%
41	8.647	1234	1240	1248	rBV	190461	298584	75.29%	9.111%
42	8.720	1249	1252	1266	rVB2	10590	21299	5.37%	0.650%
43	8.915	1282	1284	1285	rBV	340	268	0.07%	0.008%
44	8.952	1285	1290	1297	rBV2	30717	47327	11.93%	1.444%
45	9.159	1320	1324	1328	rVB2	294	601	0.15%	0.018%
46	9.275	1338	1343	1348	rBV3	1616	1864	0.47%	0.057%
47	9.330	1350	1352	1354	rVB	346	294	0.07%	0.009%
48	9.397	1357	1363	1374	rBV	89768	188002	47.40%	5.737%
49	9.641	1402	1403	1404	rBV	355	254	0.06%	0.008%
50	9.671	1406	1408	1411	rVB3	1210	1250	0.32%	0.038%
51	9.756	1419	1422	1428	rVB3	1795	2442	0.62%	0.075%
52	9.836	1431	1435	1436	rBV	774	576	0.15%	0.018%
53	9.909	1444	1447	1451	rVB3	1246	1590	0.40%	0.049%
54	9.945	1451	1453	1457	rVB2	540	856	0.22%	0.026%
55	10.013	1457	1464	1466	rBV4	2289	3915	0.99%	0.119%
56	10.055	1466	1471	1482	rVB	260719	360860	90.99%	11.012%
57	10.208	1492	1496	1498	rBV2	646	860	0.22%	0.026%
58	10.244	1498	1502	1508	rVB4	1421	2508	0.63%	0.077%
59	10.311	1508	1513	1516	rBV4	880	1407	0.35%	0.043%
60	10.409	1525	1529	1532	rVB2	897	1216	0.31%	0.037%
61	10.567	1553	1555	1558	rVB2	322	352	0.09%	0.011%
62	10.598	1558	1560	1563	rBV	336	464	0.12%	0.014%
63	10.647	1565	1568	1569	rBV2	431	447	0.11%	0.014%
64	10.903	1607	1610	1612	rBV	327	438	0.11%	0.013%
65	10.921	1612	1613	1617	rBV2	173	255	0.06%	0.008%
66	11.195	1652	1658	1667	rBV	151023	207978	52.44%	6.346%
67	11.348	1682	1683	1688	rVB	246	330	0.08%	0.010%
68	11.402	1689	1692	1696	rBV	420	671	0.17%	0.020%
69	11.738	1744	1747	1750	rVV	326	425	0.11%	0.013%
70	11.799	1755	1757	1762	rVB2	492	566	0.14%	0.017%
71	12.024	1788	1794	1804	rVV	241795	308066	77.68%	9.401%
72	12.110	1807	1808	1811	rBV3	439	360	0.09%	0.011%
73	12.177	1816	1819	1820	rBV	244	252	0.06%	0.008%
74	12.317	1837	1842	1850	rBV	194236	260853	65.77%	7.960%
75	12.762	1913	1915	1919	rVB2	582	619	0.16%	0.019%
76	12.908	1938	1939	1943	rBV2	311	380	0.10%	0.012%

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Sample : P3344-03ME
Misc : 4.76g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : BHB19ME

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_X\Method\SFAMXLM072624WMA.M
Title : VOC Analysis

77	13.024	1957	1958	1963	rVB2	335	420	0.11%	0.013%
78	13.207	1985	1988	1990	rBV3	320	377	0.10%	0.012%
79	13.433	2024	2025	2028	rBV	251	249	0.06%	0.008%
80	13.579	2043	2049	2055	rBV	276	679	0.17%	0.021%
81	13.713	2069	2071	2075	rVB2	377	361	0.09%	0.011%
82	14.006	2114	2119	2121	rBV	176	307	0.08%	0.009%
83	14.128	2137	2139	2143	rVB	642	685	0.17%	0.021%
84	14.311	2167	2169	2171	rBV	228	262	0.07%	0.008%
85	14.432	2187	2189	2192	rVB2	531	579	0.15%	0.018%
86	14.597	2210	2216	2218	rBV2	462	652	0.16%	0.020%
87	14.762	2241	2243	2244	rBV	252	269	0.07%	0.008%
88	14.829	2251	2254	2257	rBV3	275	367	0.09%	0.011%
89	14.981	2277	2279	2282	rBV2	272	251	0.06%	0.008%
90	15.146	2302	2306	2310	rVB3	789	919	0.23%	0.028%
91	15.231	2315	2320	2326	rVB2	33958	49700	12.53%	1.517%
92	15.396	2342	2347	2351	rBV4	558	1084	0.27%	0.033%
93	15.481	2360	2361	2364	rVV	502	359	0.09%	0.011%
94	15.518	2364	2367	2370	rVV	640	674	0.17%	0.021%
95	15.731	2397	2402	2408	rVB2	15797	24025	6.06%	0.733%
96	15.914	2428	2432	2435	rBV3	348	408	0.10%	0.012%
97	15.963	2435	2440	2444	rBV5	2183	3426	0.86%	0.105%
98	16.091	2455	2461	2468	rBV2	24468	40179	10.13%	1.226%
99	16.194	2473	2478	2479	rVB3	646	906	0.23%	0.028%
100	16.414	2510	2514	2516	rBV3	260	380	0.10%	0.012%

Sum of corrected areas: 3277055

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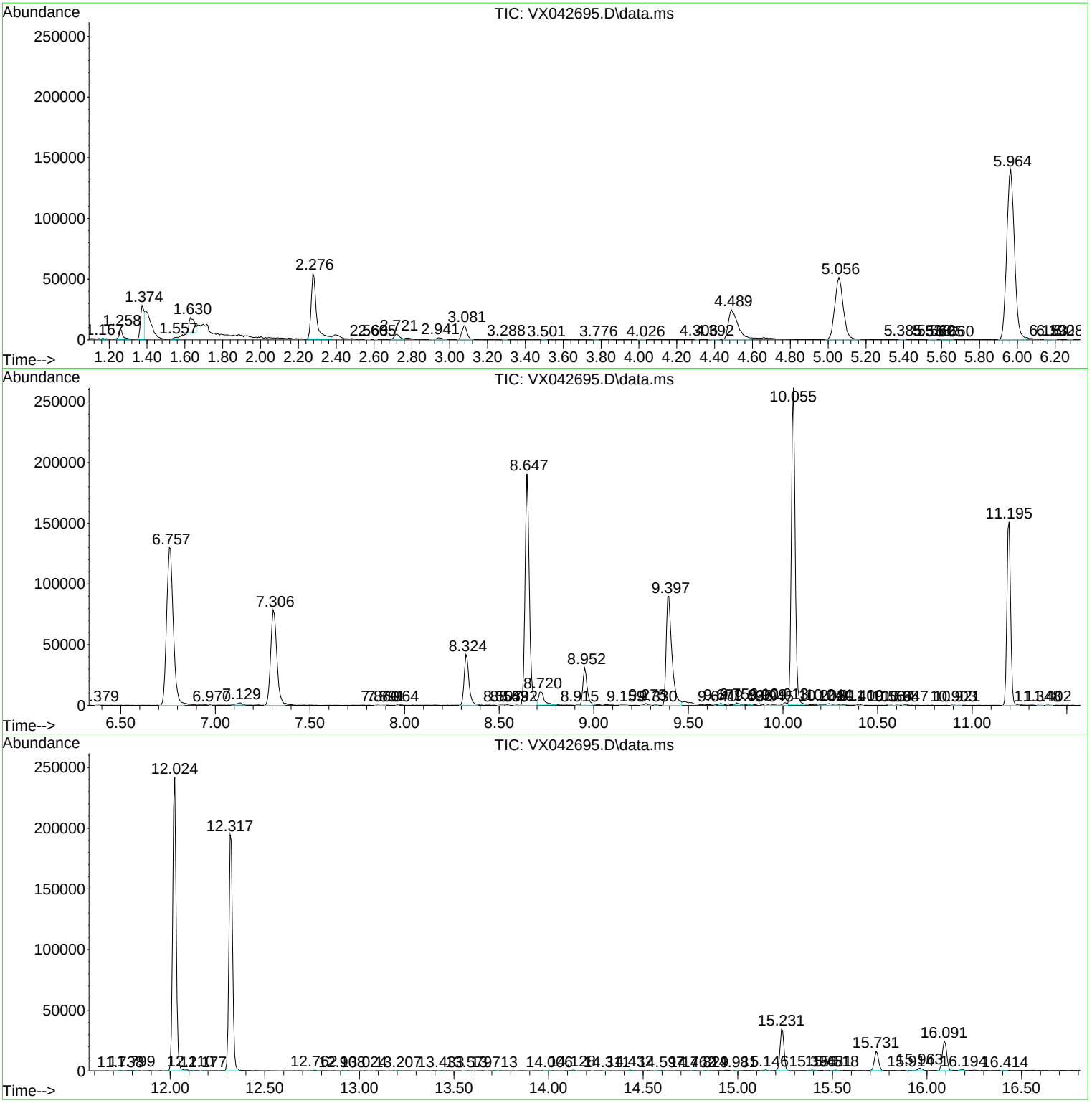
Sample : P3344-03ME
Misc : 4.76g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BHB19ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072924\
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Instrument :
MSVOA_X
ClientSampleId :
BHB19ME

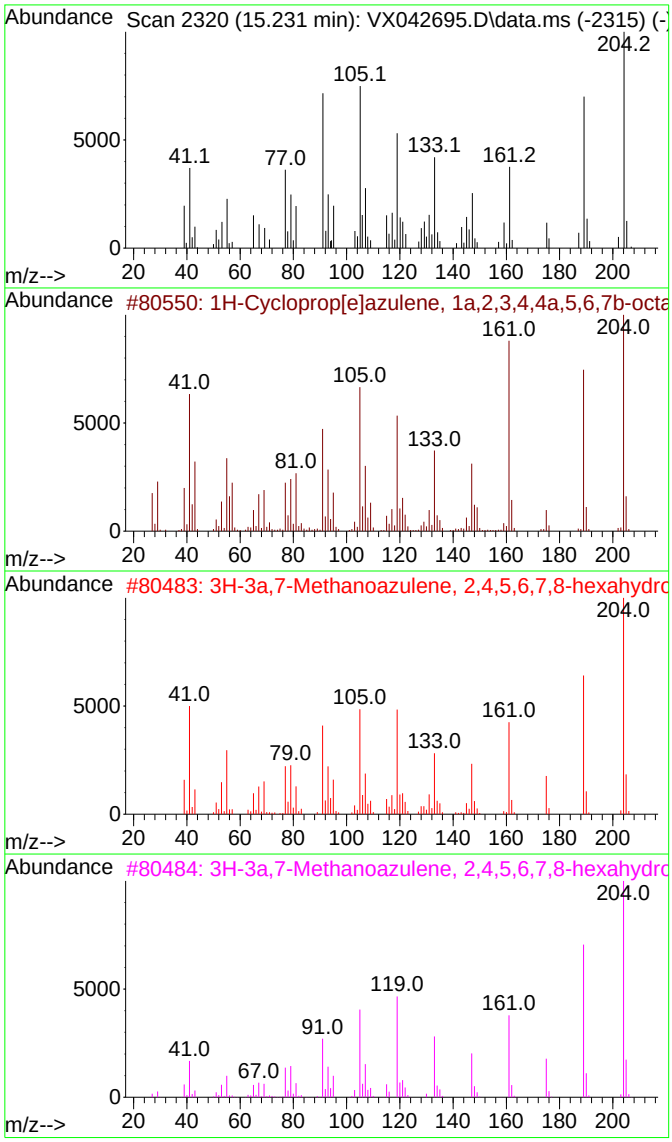
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

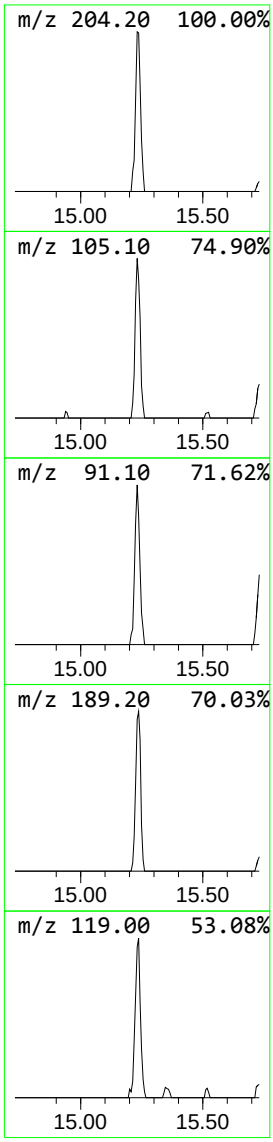
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1H-Cycloprop[e]azulene, 1a,... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.231	8.07 ug/L	49700	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Cycloprop[e]azulene, 1a,2,3,4...	204	C15H24	000489-40-7	93
2	3H-3a,7-Methanoazulene, 2,4,5,6,...	204	C15H24	002387-78-2	91
3	3H-3a,7-Methanoazulene, 2,4,5,6,...	204	C15H24	002387-78-2	90
4	1H-Cycloprop[e]azulene, 1a,2,3,4...	204	C15H24	000489-40-7	90
5	1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	74





Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072924\
Data File : VX042695.D
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Operator : JC/MD
Sample : P3344-03ME
Misc : 4.76g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BHB19ME

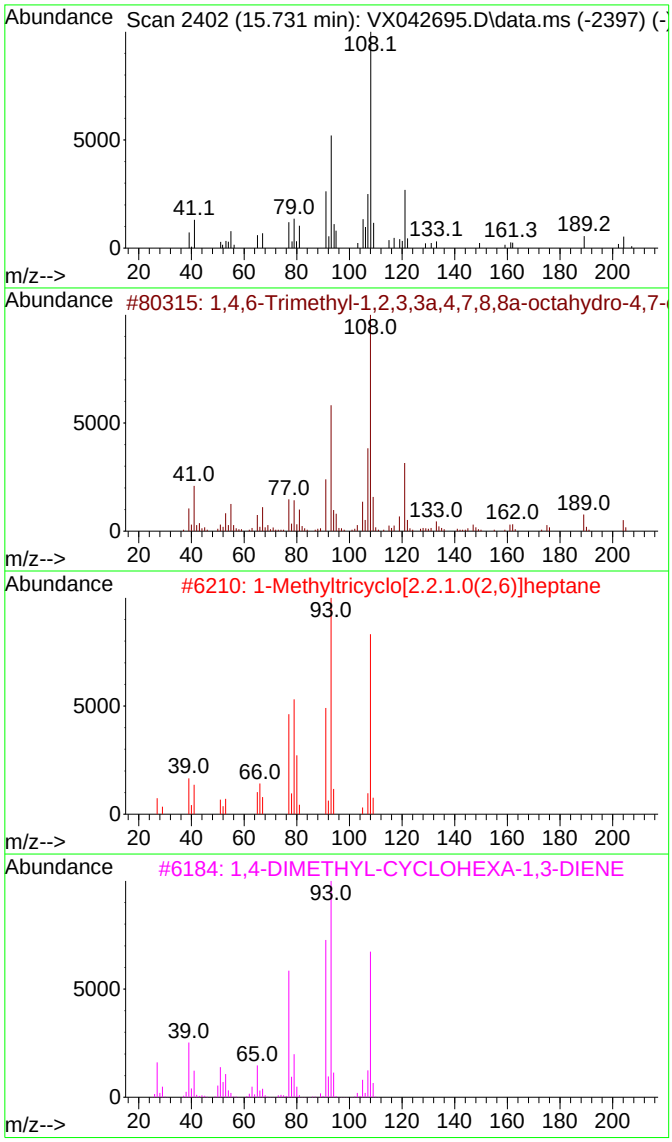
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

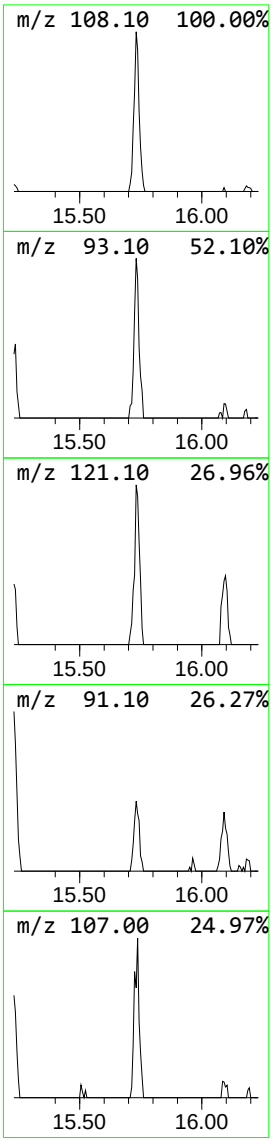
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1,4,6-Trimethyl-1,2,3,3a,4,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.731	3.90 ug/L	24025	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4,6-Trimethyl-1,2,3,3a,4,7,8,8...	204	C15H24	065128-08-7	96
2	1-Methyltricyclo[2.2.1.0(2,6)]he...	108	C8H12	004601-85-8	64
3	1,4-DIMETHYL-CYCLOHEXA-1,3-DIENE	108	C8H12	026120-52-5	59
4	Cyclopentene, 3-ethylidene-1-met...	108	C8H12	062338-00-5	59
5	(E,E,E)-2,4,6-Octatriene	108	C8H12	015192-80-0	58





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Instrument :
MSVOA_X
ClientSampleId :
BHB19ME

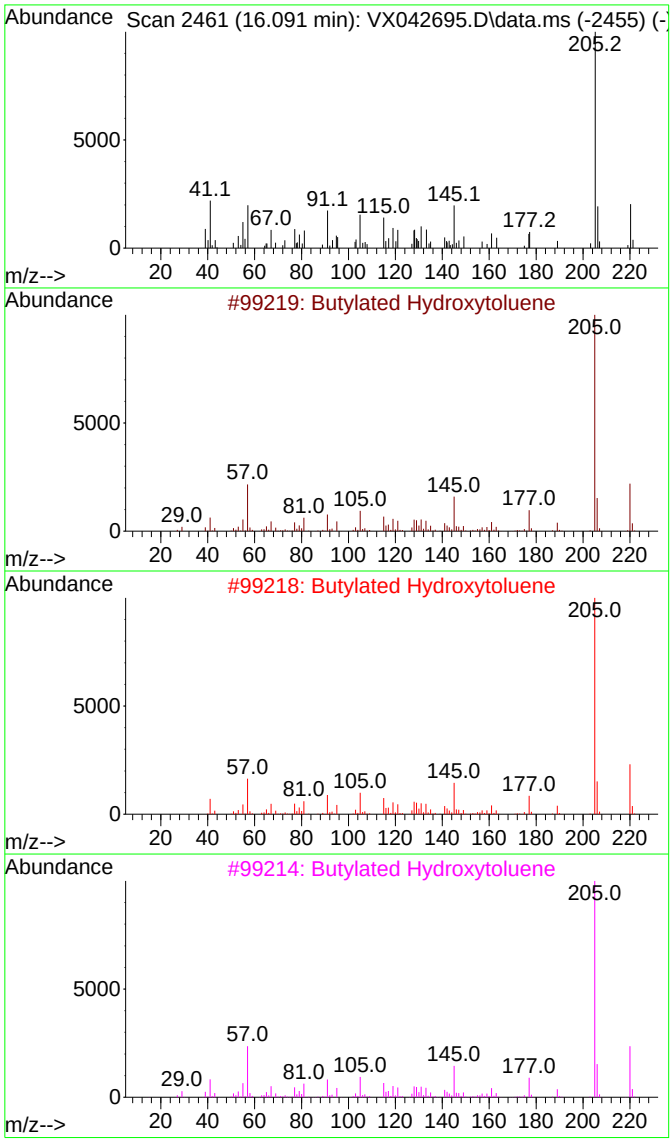
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

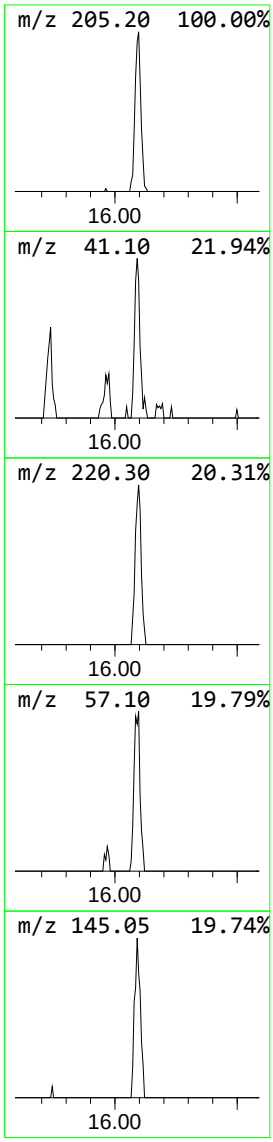
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.091	6.52 ug/L	40179	1,4-Dichlorobenzene-d4	12.024

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	96
2	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	96
3	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	95
4	Butylated Hydroxytoluene	220	C15H24O	000128-37-0	91
5	Ethyl 4-oxo-2-phenylpentanoate	220	C13H16O3	1000427-11-2	91





Tentatively Identified Compound (LSC) summary

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Instrument :
MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.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
1H-Cycloprop[e]...	15.231	8.1	ug/L	49700	3	12.024	308066	50.0
1,4,6-Trimethyl...	15.731	3.9	ug/L	24025	3	12.024	308066	50.0
Butylated Hydro...	16.091	6.5	ug/L	40179	3	12.024	308066	50.0