LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092623\
Data File : VV032177.D
Acq On : 26 Sep 2023 11:55
Operator : SY/MD
Sample : 04527-10ME
Misc : 5.16g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EZYY7ME

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_V\Method\SFAMVLM092523WMA.M
Title : VOC Analysis

Signal : TIC: VV032177.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.185	42	45	51	rBV	4333	3657	0.45%	0.043%
2	1.278	68	74	104	rVB	70355	112000	13.84%	1.329%
3	2.034	301	309	328	rVB	157953	232982	28.80%	2.764%
4	2.436	425	434	449	rVB2	6987	12907	1.60%	0.153%
5	2.635	494	496	499	rBV2	328	173	0.02%	0.002%
6	2.683	506	511	516	rBV5	425	501	0.06%	0.006%
7	2.709	516	519	520	rBV5	313	141	0.02%	0.002%
8	2.950	585	594	601	rVV4	948	1658	0.20%	0.020%
9	3.005	609	611	614	rBV2	197	110	0.01%	0.001%
10	3.066	627	630	632	rBV	335	204	0.03%	0.002%
11	3.133	647	651	653	rBV	138	127	0.02%	0.002%
12	3.294	698	701	705	rVB2	235	146	0.02%	0.002%
13	3.333	709	713	714	rBV	172	116	0.01%	0.001%
14	3.381	726	728	733	rBV2	186	146	0.02%	0.002%
15	3.429	742	743	748	rBV	106	103	0.01%	0.001%
16	3.503	758	766	768	rBV2	102	124	0.02%	0.001%
17	3.532	772	775	778	rBV2	188	131	0.02%	0.002%
18	3.658	810	814	820	rBV2	225	167	0.02%	0.002%
19	3.799	849	858	898	rBV2	47950	168573	20.83%	2.000%
20	4.246	981	997	1033	rBV	117535	318567	39.37%	3.779%
21	4.439	1055	1057	1064	rBV4	370	442	0.05%	0.005%
22	4.519	1080	1082	1083	rBV4	296	111	0.01%	0.001%
23	4.532	1083	1086	1089	rVB2	226	153	0.02%	0.002%
24	4.551	1089	1092	1094	rBV2	315	189	0.02%	0.002%
25	4.632	1114	1117	1118	rBV	239	147	0.02%	0.002%
26	4.658	1123	1125	1128	rVV	189	100	0.01%	0.001%
27	4.693	1132	1136	1140	rBV2	229	216	0.03%	0.003%
28	4.725	1142	1146	1150	rBV2	308	165	0.02%	0.002%
29	4.847	1182	1184	1187	rBV2	137	105	0.01%	0.001%
30	4.950	1201	1216	1253	rBV2	312708	809094	100.00%	9.597%
31	5.378	1347	1349	1351	rBV	310	159	0.02%	0.002%
32	5.410	1356	1359	1365	rBV4	297	272	0.03%	0.003%
33	5.449	1368	1371	1372	rBV4	331	205	0.03%	0.002%
34	5.484	1378	1382	1385	rBV2	233	169	0.02%	0.002%
35	5.532	1385	1397	1431	rBV	273872	598038	73.91%	7.094%
36	5.825	1478	1488	1503	rBV2	10122	23833	2.95%	0.283%

LSC Area Percent Report

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Instrument :
MSVOA_V
ClientSampleId :
EZYY7ME

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_V\Method\SFAMVLM092523WMA.M
Title : VOC Analysis

37	5.989	1527	1539	1571	rVB	172646	377299	46.63%	4.475%
38	6.339	1643	1648	1649	rBV	177	145	0.02%	0.002%
39	6.403	1665	1668	1673	rBV	167	162	0.02%	0.002%
40	6.448	1678	1682	1685	rVB	243	170	0.02%	0.002%
41	6.493	1693	1696	1700	rVB2	316	171	0.02%	0.002%
42	6.519	1701	1704	1709	rBV	133	131	0.02%	0.002%
43	6.538	1709	1710	1716	rVB2	203	129	0.02%	0.002%
44	6.590	1716	1726	1730	rBV5	778	1163	0.14%	0.014%
45	6.686	1754	1756	1759	rBV2	376	291	0.04%	0.003%
46	6.738	1770	1772	1773	rBV2	284	102	0.01%	0.001%
47	6.844	1797	1805	1813	rBV4	1009	1800	0.22%	0.021%
48	6.915	1816	1827	1850	rBV	94285	189804	23.46%	2.251%
49	7.243	1918	1929	1966	rBV	347634	633582	78.31%	7.515%
50	7.503	2003	2010	2017	rBV4	2902	3903	0.48%	0.046%
51	7.555	2017	2026	2061	rVB	61854	126240	15.60%	1.497%
52	7.764	2089	2091	2095	rBV2	176	102	0.01%	0.001%
53	7.805	2103	2104	2107	rVB2	266	107	0.01%	0.001%
54	7.908	2132	2136	2143	rVV5	978	1135	0.14%	0.013%
55	8.050	2166	2180	2212	rBV3	113509	354621	43.83%	4.206%
56	8.677	2369	2375	2376	rBV2	288	190	0.02%	0.002%
57	8.728	2381	2391	2398	rBV3	4437	7535	0.93%	0.089%
58	8.789	2398	2410	2438	rBV	410013	747192	92.35%	8.863%
59	8.953	2451	2461	2482	rVB	62452	110746	13.69%	1.314%
60	9.075	2488	2499	2514	rBV	336306	575297	71.10%	6.824%
61	9.333	2577	2579	2581	rVB	278	131	0.02%	0.002%
62	9.413	2593	2604	2612	rBV8	3134	5816	0.72%	0.069%
63	9.484	2615	2626	2648	rVV	136499	232518	28.74%	2.758%
64	9.735	2698	2704	2710	rBV6	2127	3173	0.39%	0.038%
65	9.818	2727	2730	2737	rBV2	336	302	0.04%	0.004%
66	9.850	2737	2740	2741	rBV2	274	170	0.02%	0.002%
67	9.950	2766	2771	2773	rBV3	461	435	0.05%	0.005%
68	10.024	2788	2794	2796	rBV3	531	582	0.07%	0.007%
69	10.159	2823	2836	2853	rBV	231474	394681	48.78%	4.682%
70	10.397	2902	2910	2929	rBV2	4494	10082	1.25%	0.120%
71	10.570	2961	2964	2969	rBV	200	144	0.02%	0.002%
72	10.651	2986	2989	2990	rBV	218	106	0.01%	0.001%
73	10.664	2991	2993	2995	rBV2	487	290	0.04%	0.003%
74	10.863	3047	3055	3065	rBV	6787	9758	1.21%	0.116%
75	10.940	3076	3079	3085	rVB2	231	201	0.02%	0.002%
76	11.008	3098	3100	3104	rVB2	376	253	0.03%	0.003%

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Instrument :
MSVOA_V
ClientSampleId :
EZYY7ME

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_V\Method\SFAMVLM092523WMA.M
Title : VOC Analysis

77	11.033	3104	3108	3110	rBV2	170	114	0.01%	0.001%
78	11.098	3125	3128	3131	rVB2	283	207	0.03%	0.002%
79	11.136	3133	3140	3146	rBV4	916	1220	0.15%	0.014%
80	11.191	3146	3157	3178	rBV	521207	802020	99.13%	9.513%
81	11.323	3196	3198	3203	rBV4	571	423	0.05%	0.005%
82	11.464	3239	3242	3244	rBV3	256	191	0.02%	0.002%
83	11.493	3249	3251	3255	rVB	240	110	0.01%	0.001%
84	11.519	3255	3259	3262	rBV3	329	290	0.04%	0.003%
85	11.567	3262	3274	3295	rBV	403307	631132	78.00%	7.486%
86	11.738	3319	3327	3333	rBV5	1351	2158	0.27%	0.026%
87	11.869	3366	3368	3370	rBV2	298	166	0.02%	0.002%
88	12.410	3533	3536	3541	rVB2	442	354	0.04%	0.004%
89	12.432	3541	3543	3547	rBV3	294	226	0.03%	0.003%
90	12.451	3547	3549	3552	rVV	249	149	0.02%	0.002%
91	12.529	3570	3573	3574	rBV	248	141	0.02%	0.002%
92	12.586	3588	3591	3594	rBV3	421	371	0.05%	0.004%
93	13.448	3851	3859	3872	rBV	10950	17722	2.19%	0.210%
94	13.689	3929	3934	3942	rBV4	1440	1802	0.22%	0.021%
95	13.837	3977	3980	3982	rBV3	768	537	0.07%	0.006%
96	14.966	4323	4331	4340	rBV4	9066	14722	1.82%	0.175%
97	15.281	4419	4429	4444	rBV	41253	68254	8.44%	0.810%
98	15.422	4464	4473	4481	rBV2	19231	29044	3.59%	0.345%
99	15.535	4497	4508	4532	rVB	239651	384110	47.47%	4.556%
100	16.104	4675	4685	4694	rBV	247223	398395	49.24%	4.726%

Sum of corrected areas: 8430448

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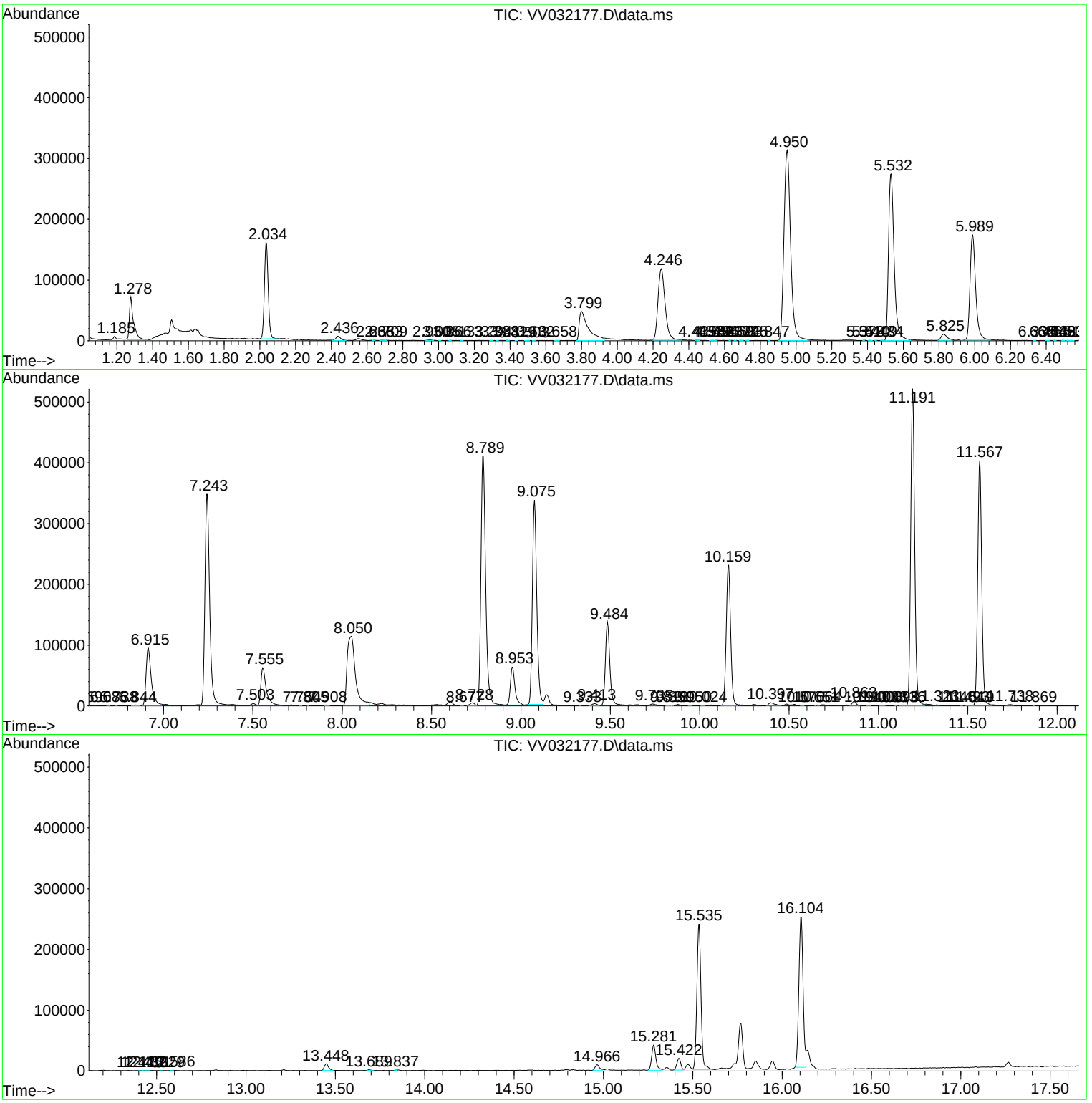
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EZYY7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092523WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092623\
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Instrument :
MSVOA_V
ClientSampleId :
EZYY7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092523WMA.M
Quant Title : VOC Analysis

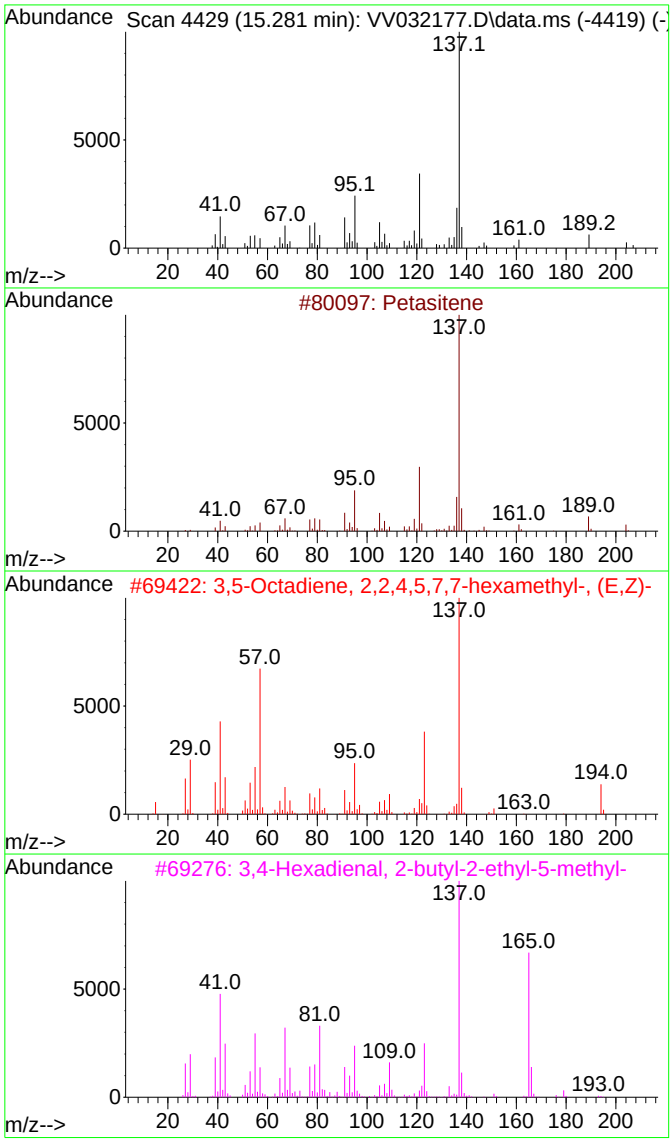
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

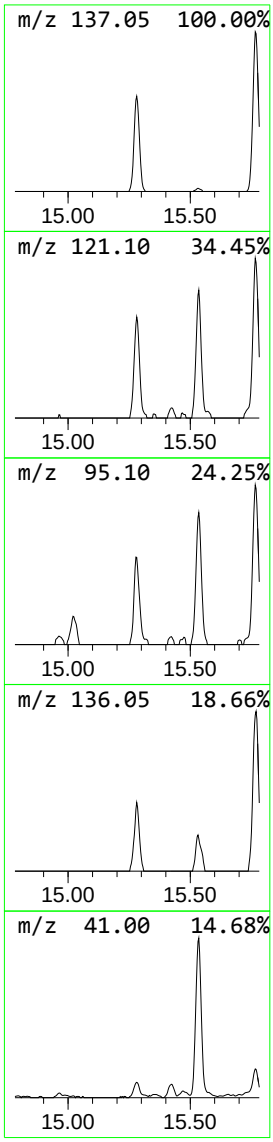
****

Peak Number 2 Petasitene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.281	4.26 ug/L	68254	1,4-Dichlorobenzene-d4	11.191

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Petasitene	204	C15H24	443124-67-2	97
2	3,5-Octadiene, 2,2,4,5,7,7-hexam...	194	C14H26	055712-52-2	72
3	3,4-Hexadienal, 2-butyl-2-ethyl-...	194	C13H22O	023739-80-2	64
4	3,3-Dimethoxy-6,6-dimethyl-cyclo...	168	C10H16O2	1010186-49-1	53
5	1,3-Benzodioxol-5-amine	137	C7H7NO2	014268-66-7	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092623\
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Acq On : 26 Sep 2023 11:55
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Misc : 5.16g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EZYY7ME

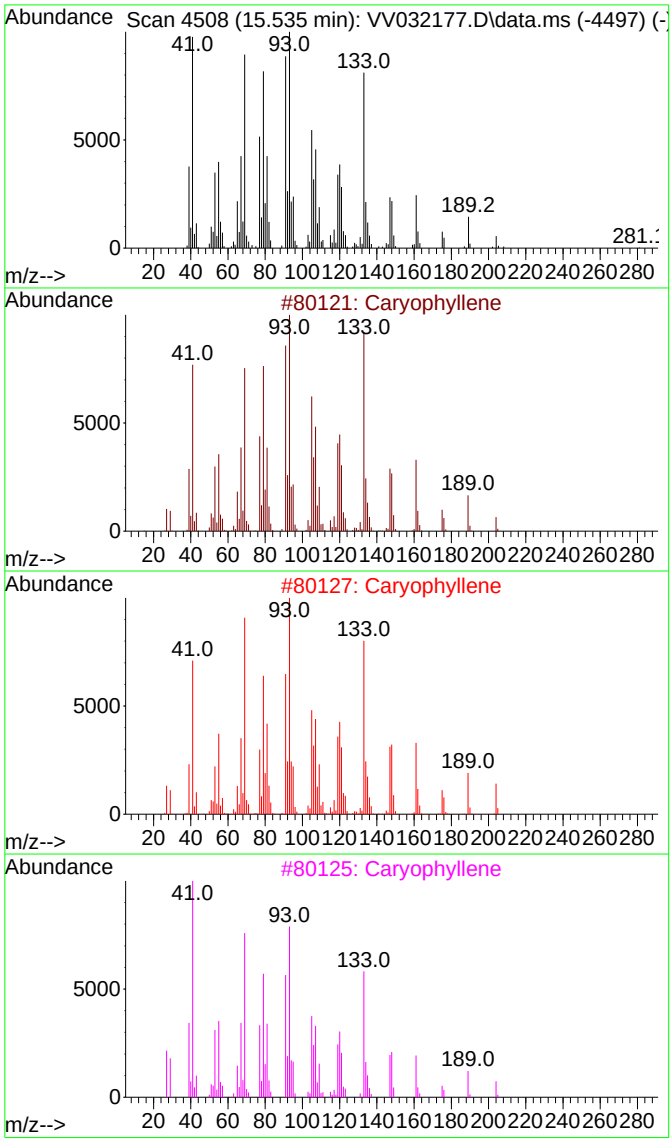
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092523WMA.M
Quant Title : VOC Analysis

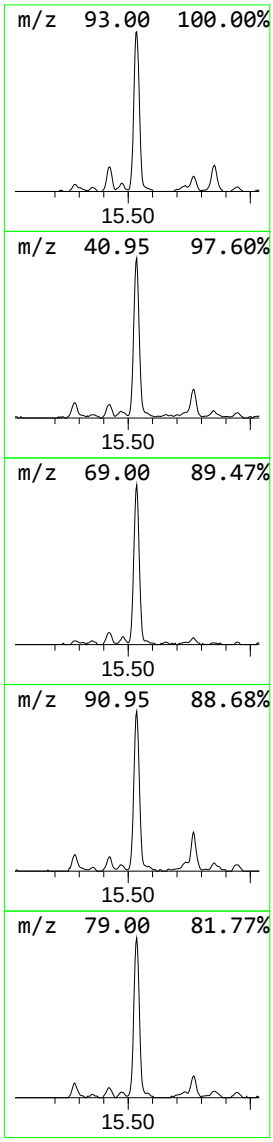
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Caryophyllene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.535	23.95 ug/L	384110	1,4-Dichlorobenzene-d4	11.191

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caryophyllene	204	C15H24	000087-44-5	99
2	Caryophyllene	204	C15H24	000087-44-5	99
3	Caryophyllene	204	C15H24	000087-44-5	99
4	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	98
5	Caryophyllene	204	C15H24	000087-44-5	96





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ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
EZYY7ME

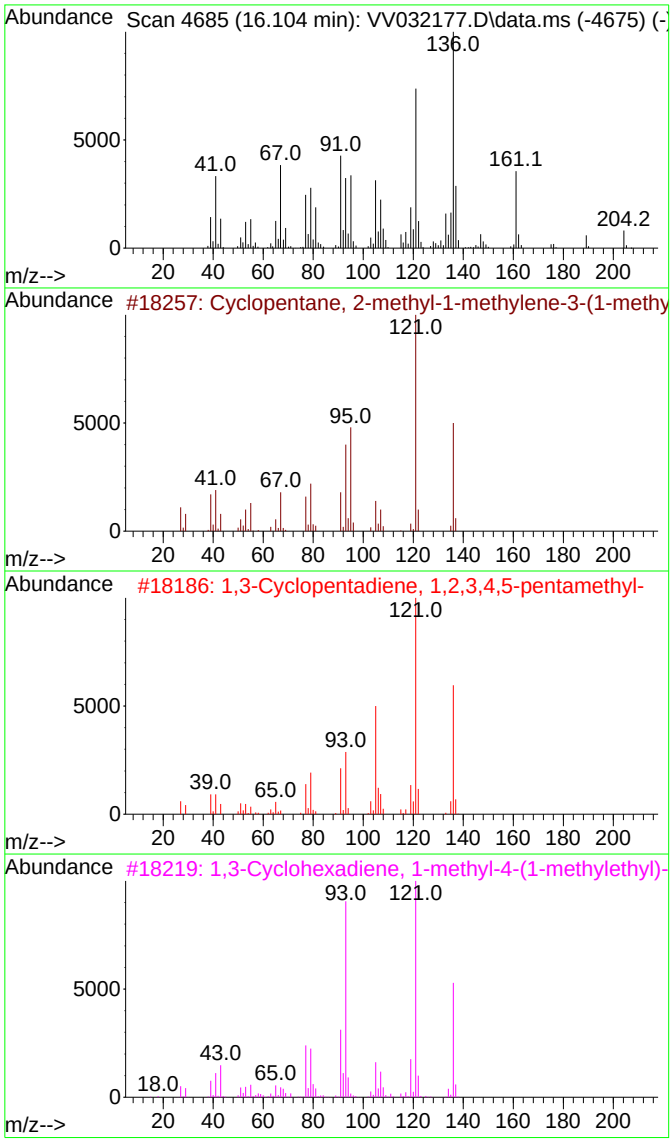
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092523WMA.M
Quant Title : VOC Analysis

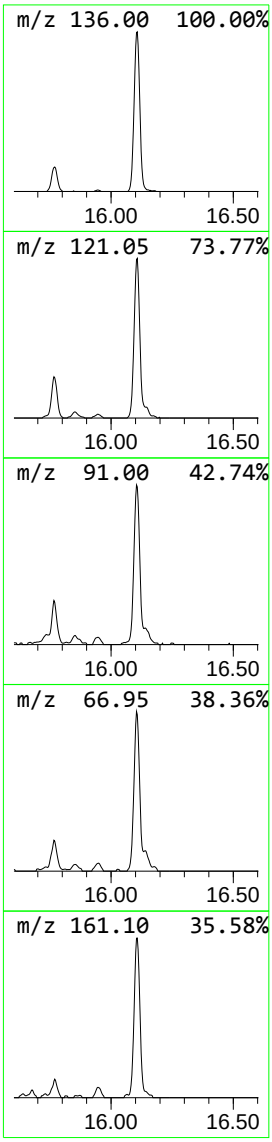
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentane, 2-methyl-1-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.104	24.84 ug/L	398395	1,4-Dichlorobenzene-d4	11.191

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 2-methyl-1-methyle...	136	C10H16	056710-83-9	64
2	1,3-Cyclopentadiene, 1,2,3,4,5-p...	136	C10H16	004045-44-7	60
3	1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	60
4	3,4-Dimethylanisole	136	C9H12O	004685-47-6	55
5	3-Ethylanisole	136	C9H12O	010568-38-4	53





Tentatively Identified Compound (LSC) summary

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MSVOA_V
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM092523WMA.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
Petasitene	15.281	4.3	ug/L	68254	3	11.191	802020	50.0
Caryophyllene	15.535	23.9	ug/L	384110	3	11.191	802020	50.0
Cyclopentane, 2...	16.104	24.8	ug/L	398395	3	11.191	802020	50.0