

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092023\
 Data File : VV032146.D
 Acq On : 20 Sep 2023 14:46
 Operator : SY/MD
 Sample : 04472-04ME
 Misc : 3.69g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 EZYK8ME

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\SFAMVLM082323WMA.M

Title : VOC Analysis

Signal : TIC: VV032146.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	40	45	50	rBV2	9410	8814	1.11%	0.138%
2	1.275	67	73	96	rVB	74219	111826	14.04%	1.748%
3	2.034	301	309	332	rVB	156026	225969	28.37%	3.531%
4	2.722	521	523	525	rBV	412	156	0.02%	0.002%
5	2.738	525	528	532	rVB2	461	356	0.04%	0.006%
6	2.838	557	559	560	rBV	627	278	0.03%	0.004%
7	2.921	581	585	587	rBV3	446	419	0.05%	0.007%
8	3.018	613	615	617	rVB2	471	179	0.02%	0.003%
9	3.031	617	619	626	rBV	318	348	0.04%	0.005%
10	3.069	627	631	632	rBV3	301	179	0.02%	0.003%
11	3.208	670	674	678	rVB2	256	264	0.03%	0.004%
12	3.294	696	701	703	rBV2	241	211	0.03%	0.003%
13	3.571	784	787	790	rBV3	244	178	0.02%	0.003%
14	3.609	796	799	803	rBV	251	162	0.02%	0.003%
15	3.638	803	808	809	rBV	654	460	0.06%	0.007%
16	3.806	851	860	897	rBV	39346	138175	17.35%	2.159%
17	4.162	969	971	976	rBV2	358	283	0.04%	0.004%
18	4.249	981	998	1029	rBV	101216	278830	35.00%	4.357%
19	4.757	1154	1156	1159	rBV	208	140	0.02%	0.002%
20	4.809	1165	1172	1177	rBV5	854	1036	0.13%	0.016%
21	4.953	1201	1217	1246	rBV2	285147	724167	90.91%	11.317%
22	5.535	1386	1398	1426	rBV	270334	587237	73.72%	9.177%
23	5.828	1479	1489	1501	rBV3	8624	19634	2.46%	0.307%
24	5.989	1528	1539	1578	rVB	151394	353992	44.44%	5.532%
25	6.220	1607	1611	1614	rBV3	317	209	0.03%	0.003%
26	6.236	1614	1616	1619	rVV2	370	220	0.03%	0.003%
27	6.269	1622	1626	1628	rVV2	338	211	0.03%	0.003%
28	6.285	1628	1631	1635	rVV2	550	414	0.05%	0.006%
29	6.304	1635	1637	1642	rVB3	335	197	0.02%	0.003%
30	6.330	1642	1645	1648	rBV2	236	163	0.02%	0.003%
31	6.384	1660	1662	1668	rVB2	490	414	0.05%	0.006%
32	6.458	1680	1685	1687	rBV2	168	157	0.02%	0.002%
33	6.529	1703	1707	1712	rBV3	274	234	0.03%	0.004%
34	6.561	1712	1717	1719	rBV2	491	349	0.04%	0.005%
35	6.770	1779	1782	1790	rBV5	698	683	0.09%	0.011%
36	6.847	1799	1806	1816	rBV4	1079	1991	0.25%	0.031%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092023\
 Data File : VV032146.D
 Acq On : 20 Sep 2023 14:46
 Operator : SY/MD
 Sample : 04472-04ME
 Misc : 3.69g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 EZYK8ME

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\SFAMVLM082323WMA.M
 Title : VOC Analysis

37	6.918	1817	1828	1853	rBV2	81334	167583	21.04%	2.619%
38	7.130	1892	1894	1896	rBV2	308	177	0.02%	0.003%
39	7.246	1919	1930	1965	rBV	320602	589256	73.97%	9.209%
40	7.506	2002	2011	2017	rBV5	1727	2824	0.35%	0.044%
41	7.558	2019	2027	2062	rVB	54245	114119	14.33%	1.783%
42	7.831	2110	2112	2114	rBV2	281	144	0.02%	0.002%
43	7.979	2155	2158	2160	rBV3	332	202	0.03%	0.003%
44	8.053	2164	2181	2214	rBV2	101709	310148	38.93%	4.847%
45	8.500	2316	2320	2323	rBV5	1546	1633	0.20%	0.026%
46	8.603	2349	2352	2354	rBV3	965	571	0.07%	0.009%
47	8.719	2383	2388	2389	rBV3	545	456	0.06%	0.007%
48	8.789	2398	2410	2436	rBV	418012	744722	93.49%	11.638%
49	9.272	2557	2560	2562	rVB2	457	205	0.03%	0.003%
50	9.317	2572	2574	2578	rBV2	161	131	0.02%	0.002%
51	9.400	2596	2600	2602	rBV2	397	273	0.03%	0.004%
52	9.497	2620	2630	2639	rBV4	2806	4676	0.59%	0.073%
53	9.567	2650	2652	2656	rBV2	262	157	0.02%	0.002%
54	9.641	2671	2675	2676	rBV3	558	362	0.05%	0.006%
55	9.715	2693	2698	2700	rBV2	499	434	0.05%	0.007%
56	9.731	2700	2703	2704	rBV	443	265	0.03%	0.004%
57	9.796	2717	2723	2730	rVB5	677	863	0.11%	0.013%
58	9.879	2744	2749	2753	rBV2	437	512	0.06%	0.008%
59	9.928	2762	2764	2768	rBV3	255	152	0.02%	0.002%
60	10.162	2823	2837	2859	rBV	198771	339152	42.58%	5.300%
61	10.346	2892	2894	2899	rBV2	212	187	0.02%	0.003%
62	10.950	3080	3082	3085	rVB	307	154	0.02%	0.002%
63	10.969	3085	3088	3094	rBV4	635	726	0.09%	0.011%
64	11.037	3104	3109	3112	rVB2	658	523	0.07%	0.008%
65	11.088	3123	3125	3132	rVB4	810	620	0.08%	0.010%
66	11.136	3138	3140	3143	rBV2	376	279	0.04%	0.004%
67	11.191	3146	3157	3176	rBV	507153	796592	100.00%	12.449%
68	11.522	3256	3260	3262	rBV2	351	243	0.03%	0.004%
69	11.567	3262	3274	3294	rBV	350150	561722	70.52%	8.778%
70	11.735	3318	3326	3336	rBV6	3821	6071	0.76%	0.095%
71	12.027	3410	3417	3423	rBV4	383	655	0.08%	0.010%
72	12.088	3433	3436	3437	rBV2	286	179	0.02%	0.003%
73	12.140	3448	3452	3455	rBV3	209	182	0.02%	0.003%
74	12.153	3455	3456	3461	rVB3	280	164	0.02%	0.003%
75	12.259	3487	3489	3492	rVB2	425	189	0.02%	0.003%
76	12.352	3513	3518	3519	rBV3	668	514	0.06%	0.008%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092023\
 Data File : VV032146.D
 Acq On : 20 Sep 2023 14:46
 Operator : SY/MD
 Sample : 04472-04ME
 Misc : 3.69g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 EZYK8ME

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\SFAMVLM082323WMA.M
 Title : VOC Analysis

77	12.397	3530	3532	3534	rBV2	305	166	0.02%	0.003%
78	12.490	3558	3561	3566	rBV4	359	320	0.04%	0.005%
79	12.535	3572	3575	3580	rVB3	490	404	0.05%	0.006%
80	12.609	3594	3598	3601	rBV2	282	262	0.03%	0.004%
81	12.673	3614	3618	3621	rBV	286	208	0.03%	0.003%
82	12.731	3630	3636	3637	rBV2	435	337	0.04%	0.005%
83	12.802	3655	3658	3660	rBV	359	220	0.03%	0.003%
84	12.834	3660	3668	3676	rVB5	5354	7910	0.99%	0.124%
85	13.104	3750	3752	3755	rBV	339	201	0.03%	0.003%
86	13.204	3782	3783	3786	rBV3	326	185	0.02%	0.003%
87	13.262	3797	3801	3805	rBV3	500	534	0.07%	0.008%
88	13.310	3813	3816	3818	rBV2	249	169	0.02%	0.003%
89	13.368	3831	3834	3836	rBV	465	325	0.04%	0.005%
90	13.448	3854	3859	3870	rBV2	4157	5728	0.72%	0.090%
91	13.632	3913	3916	3918	rBV3	384	218	0.03%	0.003%
92	13.648	3918	3921	3923	rBV3	457	280	0.04%	0.004%
93	13.696	3930	3936	3940	rBV6	489	584	0.07%	0.009%
94	13.747	3949	3952	3953	rBV	336	149	0.02%	0.002%
95	13.847	3976	3983	3991	rVB3	6050	7711	0.97%	0.121%
96	14.165	4080	4082	4085	rBV2	371	174	0.02%	0.003%
97	14.291	4119	4121	4124	rBV2	656	335	0.04%	0.005%
98	15.281	4421	4429	4439	rBV2	14686	23554	2.96%	0.368%
99	15.535	4499	4508	4525	rVB2	88785	142285	17.86%	2.224%
100	16.104	4678	4685	4695	rBV	66722	100135	12.57%	1.565%

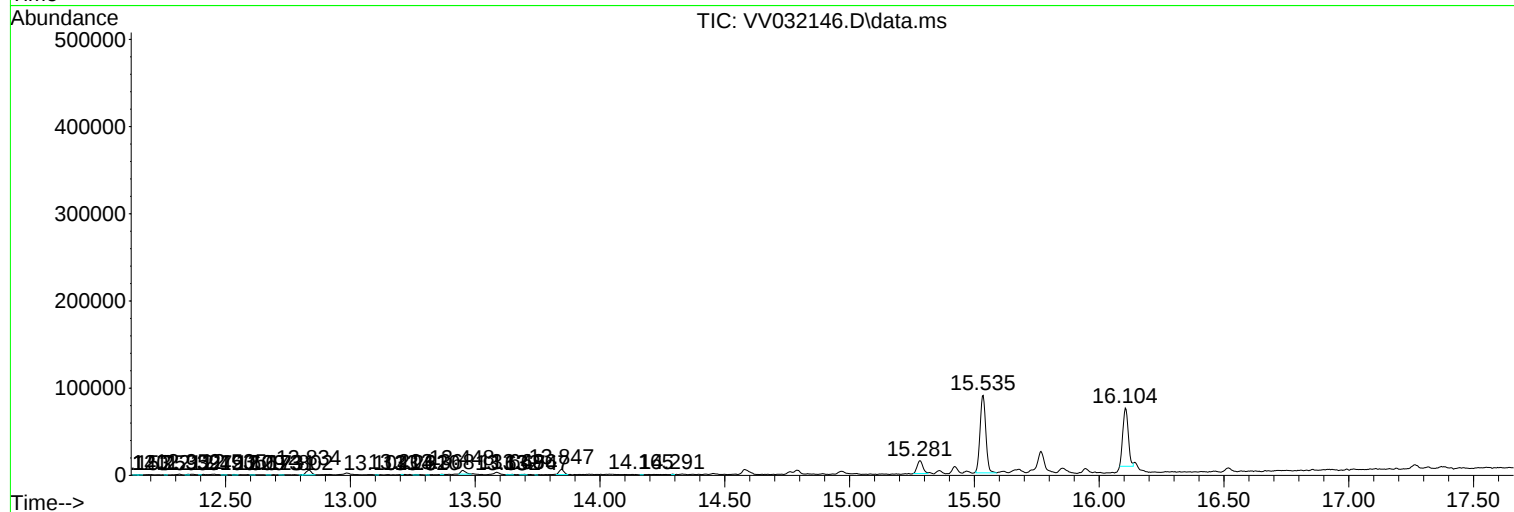
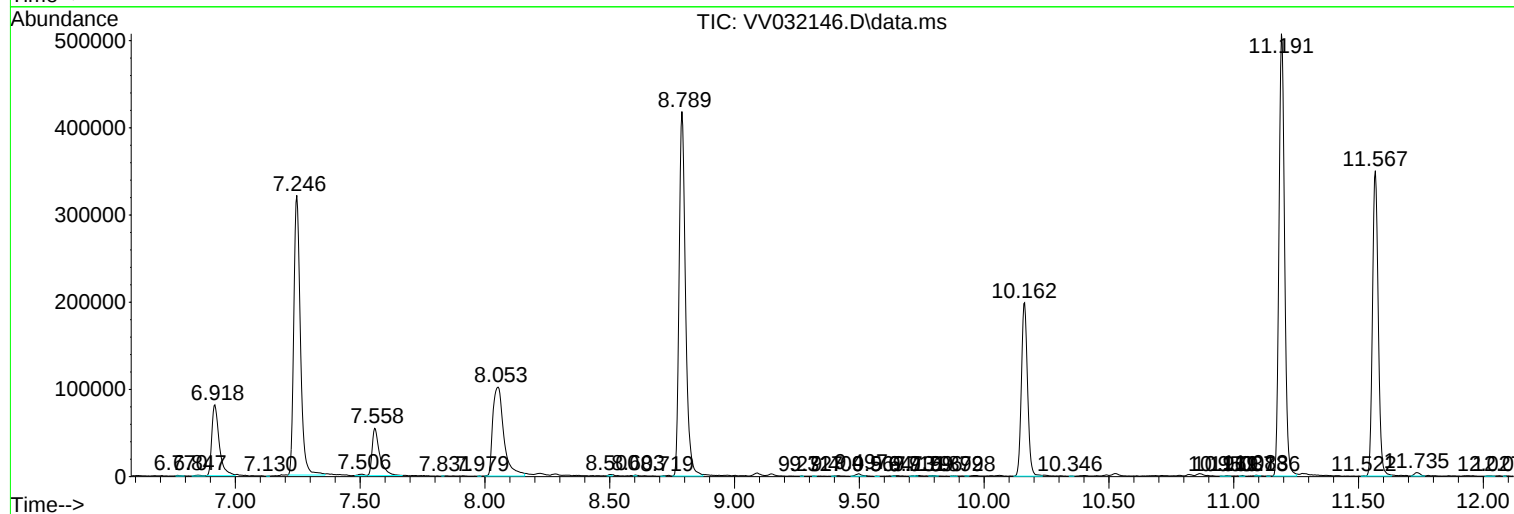
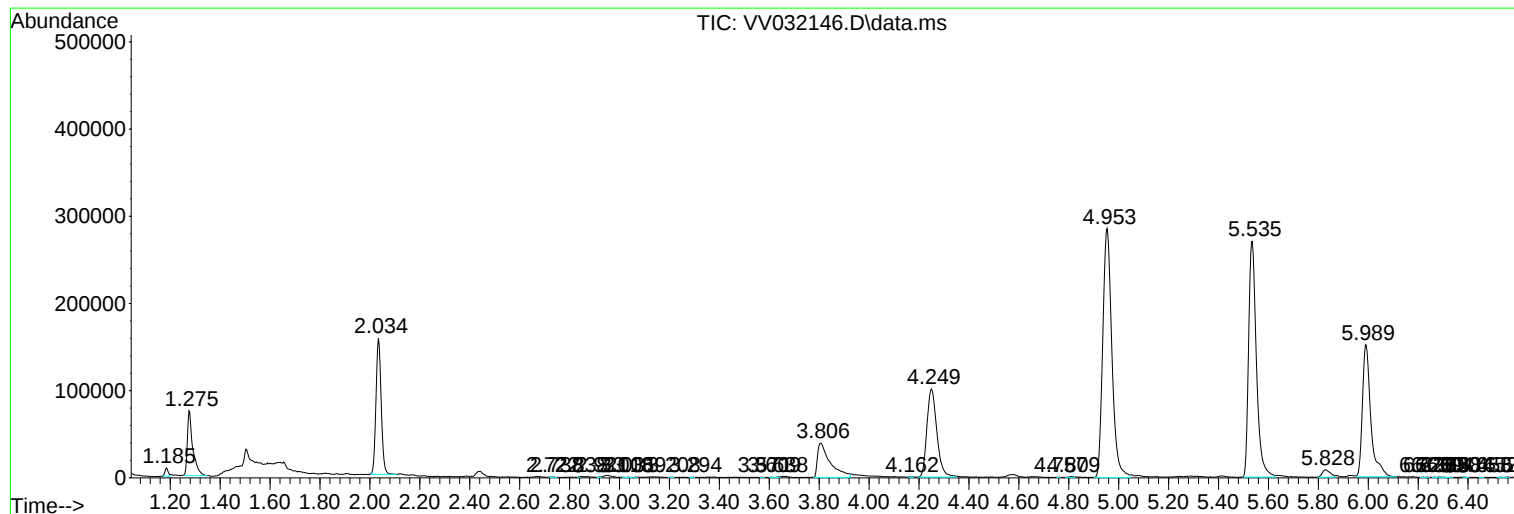
Sum of corrected areas: 6398946

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092023\
Data File : VV032146.D
Acq On : 20 Sep 2023 14:46
Operator : SY/MD
Sample : 04472-04ME
Misc : 3.69g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EZYK8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092023\
Data File : VV032146.D
Acq On : 20 Sep 2023 14:46
Operator : SY/MD
Sample : 04472-04ME
Misc : 3.69g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EZYK8ME

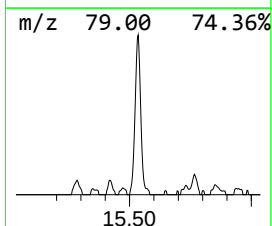
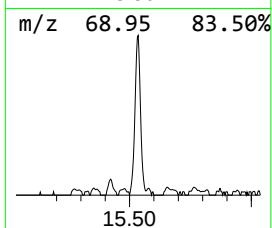
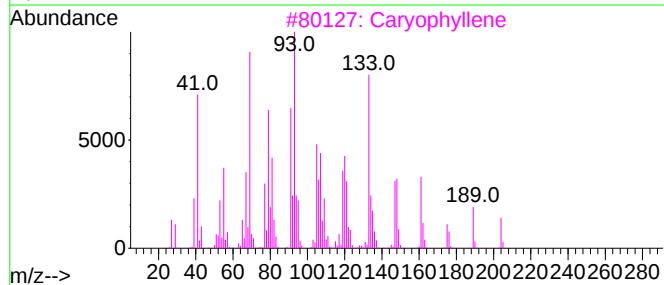
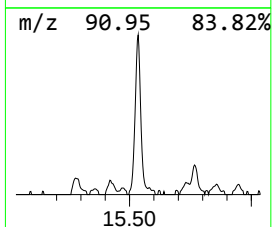
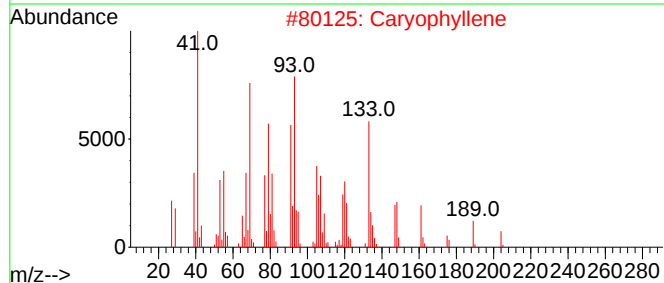
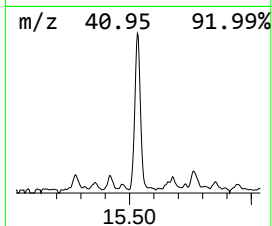
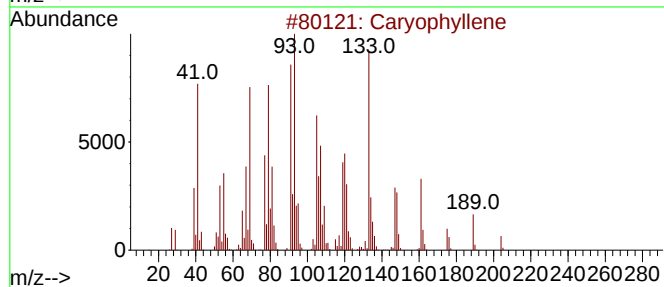
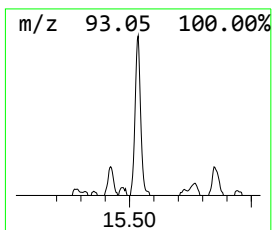
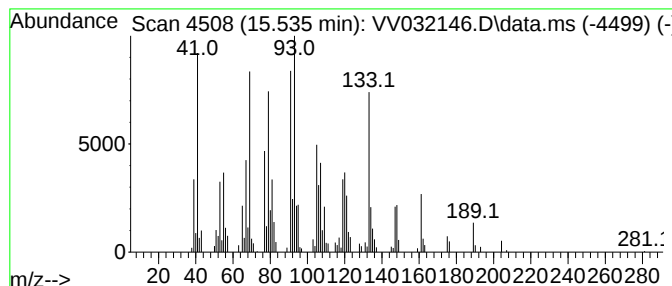
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Caryophyllene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.535	8.93 ug/L	142285	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	96
5			Caryophyllene	204	C15H24	000087-44-5	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092023\
Data File : VV032146.D
Acq On : 20 Sep 2023 14:46
Operator : SY/MD
Sample : 04472-04ME
Misc : 3.69g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EZYK8ME

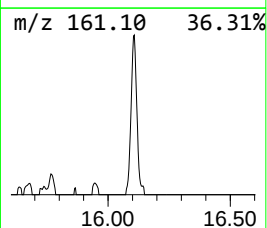
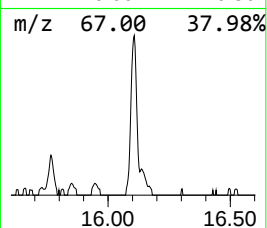
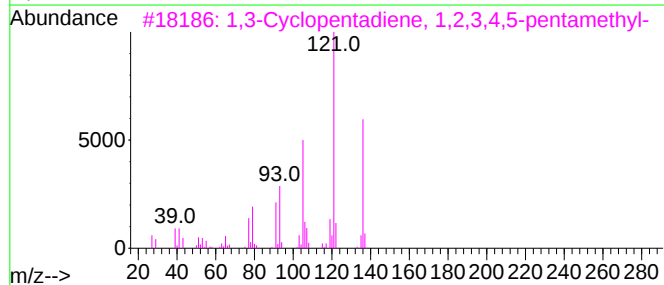
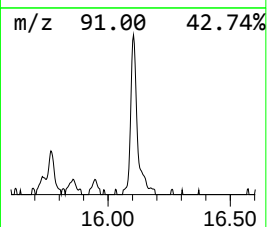
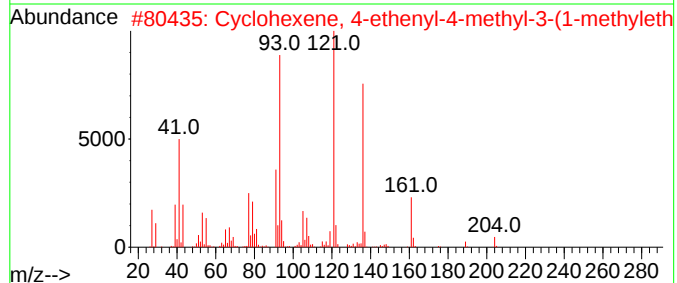
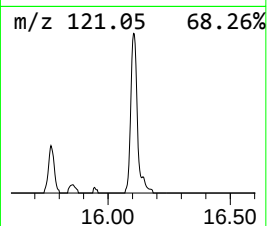
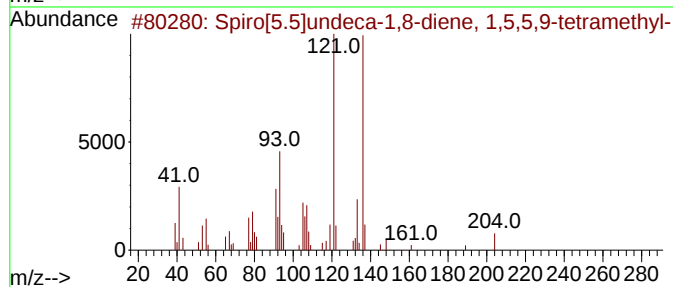
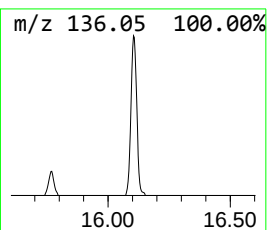
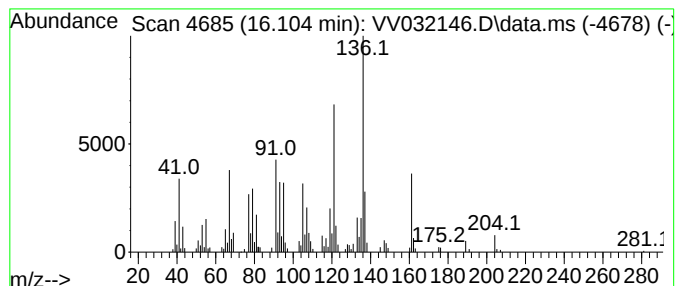
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Spiro[5.5]undeca-1,8-diene,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.104	6.29 ug/L	100135	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Spiro[5.5]undeca-1,8-diene, 1,5,...	204	C15H24	019912-83-5	80
2			Cyclohexene, 4-ethenyl-4-methyl-...	204	C15H24	020307-84-0	60
3			1,3-Cyclopentadiene, 1,2,3,4,5-p...	136	C10H16	004045-44-7	60
4			Benzenemethanol, 3,5-dimethyl-	136	C9H12O	027129-87-9	53
5			1,3-Cyclopentadiene, 1,2,3,4,5-p...	136	C10H16	004045-44-7	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV092023\
Data File : VV032146.D
Acq On : 20 Sep 2023 14:46
Operator : SY/MD
Sample : 04472-04ME
Misc : 3.69g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EZYK8ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM082323WMA.M
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
Caryophyllene	15.535	8.9	ug/L	142285	3	11.191	796592	50.0
Spiro[5.5]undec...	16.104	6.3	ug/L	100135	3	11.191	796592	50.0