

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051222\
 Data File : VU048543.D
 Acq On : 12 May 2022 15:49
 Operator : SY/MD
 Sample : N2801-08
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXLE1

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\SFAMULM050622WMA.M
 Title : VOC Analysis

Signal : TIC: VU048543.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	95	rBV	112471	123575	11.16%	1.291%
2	1.912	170	178	190	rBV	89114	114183	10.31%	1.193%
3	2.568	370	382	404	rBV	223699	369314	33.34%	3.859%
4	2.700	421	423	427	rVB	461	275	0.02%	0.003%
5	2.726	427	431	436	rBV2	301	297	0.03%	0.003%
6	3.044	518	530	547	rBV3	11946	25719	2.32%	0.269%
7	3.137	555	559	564	rVB2	399	371	0.03%	0.004%
8	3.176	567	571	572	rBV2	598	470	0.04%	0.005%
9	3.224	583	586	594	rVB2	228	287	0.03%	0.003%
10	3.260	594	597	600	rBV2	235	155	0.01%	0.002%
11	3.282	600	604	605	rBV2	343	231	0.02%	0.002%
12	3.366	617	630	642	rBV3	8831	19212	1.73%	0.201%
13	3.719	737	740	742	rBV2	296	241	0.02%	0.003%
14	3.777	754	758	759	rBV	204	143	0.01%	0.001%
15	3.816	768	770	774	rBV	320	223	0.02%	0.002%
16	3.848	774	780	783	rVV2	361	463	0.04%	0.005%
17	3.867	783	786	790	rVV2	290	252	0.02%	0.003%
18	3.893	791	794	802	rVB2	436	564	0.05%	0.006%
19	4.092	849	856	858	rBV3	435	469	0.04%	0.005%
20	4.198	884	889	892	rBV2	204	185	0.02%	0.002%
21	4.295	913	919	921	rBV	402	400	0.04%	0.004%
22	4.359	935	939	943	rBV2	329	284	0.03%	0.003%
23	4.395	946	950	954	rBV2	296	198	0.02%	0.002%
24	4.433	954	962	963	rBV3	1089	1268	0.11%	0.013%
25	4.533	978	993	1007	rBV3	16975	39877	3.60%	0.417%
26	4.616	1007	1019	1040	rBV	117439	274851	24.81%	2.872%
27	4.996	1135	1137	1140	rBV2	318	126	0.01%	0.001%
28	5.067	1142	1159	1176	rBV	207227	459461	41.48%	4.800%
29	5.189	1194	1197	1199	rBV3	582	452	0.04%	0.005%
30	5.240	1210	1213	1215	rVB	356	188	0.02%	0.002%
31	5.263	1218	1220	1222	rVB	276	147	0.01%	0.002%
32	5.292	1222	1229	1237	rBV3	628	1016	0.09%	0.011%
33	5.394	1245	1261	1273	rBV4	13631	31247	2.82%	0.326%
34	5.462	1273	1282	1300	rVB9	5130	11285	1.02%	0.118%
35	5.539	1302	1306	1309	rBV	367	281	0.03%	0.003%
36	5.571	1312	1316	1317	rBV	303	200	0.02%	0.002%

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Integrator: RTE

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
 Title : VOC Analysis

37	5.591	1317	1322	1323	rBV2	488	430	0.04%	0.004%
38	5.639	1328	1337	1343	rBV6	1421	2703	0.24%	0.028%
39	5.726	1343	1364	1383	rBV2	406134	1107758	100.00%	11.574%
40	6.038	1459	1461	1464	rBV3	559	337	0.03%	0.004%
41	6.160	1497	1499	1502	rVB	351	195	0.02%	0.002%
42	6.185	1503	1507	1510	rBV	149	165	0.01%	0.002%
43	6.250	1512	1527	1552	rBV	331830	632281	57.08%	6.606%
44	6.459	1589	1592	1595	rBV2	483	405	0.04%	0.004%
45	6.526	1606	1613	1623	rBV6	2767	5262	0.48%	0.055%
46	6.690	1651	1664	1681	rBV	254008	497971	44.95%	5.203%
47	6.906	1726	1731	1734	rBV	388	324	0.03%	0.003%
48	6.970	1749	1751	1753	rVV	630	298	0.03%	0.003%
49	6.983	1753	1755	1759	rVB2	276	182	0.02%	0.002%
50	7.166	1802	1812	1813	rBV7	1264	1623	0.15%	0.017%
51	7.250	1836	1838	1839	rBV7	334	187	0.02%	0.002%
52	7.285	1846	1849	1855	rVB2	275	395	0.04%	0.004%
53	7.314	1855	1858	1861	rBV2	434	322	0.03%	0.003%
54	7.391	1871	1882	1892	rVV6	4999	9573	0.86%	0.100%
55	7.568	1923	1937	1962	rBV	144823	261375	23.59%	2.731%
56	7.812	2011	2013	2021	rVB2	160	164	0.01%	0.002%
57	7.899	2026	2040	2056	rBV	513653	879649	79.41%	9.191%
58	8.179	2115	2127	2145	rBV	110995	187346	16.91%	1.957%
59	8.410	2191	2199	2209	rBV5	1533	2478	0.22%	0.026%
60	8.546	2237	2241	2242	rVV	310	179	0.02%	0.002%
61	8.558	2242	2245	2249	rVB2	512	345	0.03%	0.004%
62	8.632	2256	2268	2294	rBV	348997	638903	57.68%	6.675%
63	8.992	2376	2380	2383	rBV2	382	268	0.02%	0.003%
64	9.012	2383	2386	2392	rVV	247	214	0.02%	0.002%
65	9.369	2493	2497	2499	rBV2	268	208	0.02%	0.002%
66	9.417	2499	2512	2532	rBV	479201	803034	72.49%	8.390%
67	9.568	2553	2559	2578	rVB4	9663	14824	1.34%	0.155%
68	9.639	2578	2581	2583	rBV3	394	234	0.02%	0.002%
69	9.867	2649	2652	2655	rVB	218	121	0.01%	0.001%
70	9.944	2673	2676	2678	rBV	291	165	0.01%	0.002%
71	10.102	2717	2725	2742	rVB3	5578	8846	0.80%	0.092%
72	10.417	2820	2823	2826	rBV	229	159	0.01%	0.002%
73	10.484	2834	2844	2854	rVB2	14750	21931	1.98%	0.229%
74	10.581	2871	2874	2877	rBV	160	133	0.01%	0.001%
75	10.629	2888	2889	2892	rVB2	311	154	0.01%	0.002%
76	10.645	2892	2894	2896	rBV	282	154	0.01%	0.002%

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Integration Parameters: LSCINT.P

Integrator: RTE

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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 >

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
 Title : VOC Analysis

77	10.758	2916	2929	2951	rVV	377551	612514	55.29%	6.400%
78	10.906	2965	2975	2989	rVB2	23385	38429	3.47%	0.402%
79	11.121	3038	3042	3046	rBV2	395	397	0.04%	0.004%
80	11.291	3084	3095	3111	rVB	136183	214303	19.35%	2.239%
81	11.468	3140	3150	3163	rVB	21944	34210	3.09%	0.357%
82	11.516	3163	3165	3169	rBV	199	127	0.01%	0.001%
83	11.690	3216	3219	3222	rBV3	851	615	0.06%	0.006%
84	11.745	3230	3236	3244	rVB5	2682	2954	0.27%	0.031%
85	11.812	3244	3257	3273	rBV	544759	865067	78.09%	9.038%
86	12.095	3331	3345	3362	rBV5	42585	74877	6.76%	0.782%
87	12.192	3362	3375	3391	rBV	561197	908473	82.01%	9.492%
88	12.304	3403	3410	3424	rVB7	4921	7631	0.69%	0.080%
89	12.375	3425	3432	3444	rVB2	10920	15794	1.43%	0.165%
90	12.465	3452	3460	3475	rVB2	12861	19001	1.72%	0.199%
91	12.571	3484	3493	3502	rBV	31281	46509	4.20%	0.486%
92	12.680	3518	3527	3545	rVB3	31711	53915	4.87%	0.563%
93	12.767	3549	3554	3558	rBV4	605	707	0.06%	0.007%
94	12.973	3608	3618	3630	rBV	23479	36240	3.27%	0.379%
95	13.298	3711	3719	3728	rVB5	9316	13510	1.22%	0.141%
96	13.455	3759	3768	3781	rVB2	25204	38098	3.44%	0.398%
97	13.526	3782	3790	3797	rBV4	3003	4031	0.36%	0.042%
98	13.629	3815	3822	3832	rVB6	4187	6595	0.60%	0.069%
99	13.770	3862	3866	3867	rBV2	1009	589	0.05%	0.006%
100	14.092	3958	3966	3975	rVB2	11903	17434	1.57%	0.182%

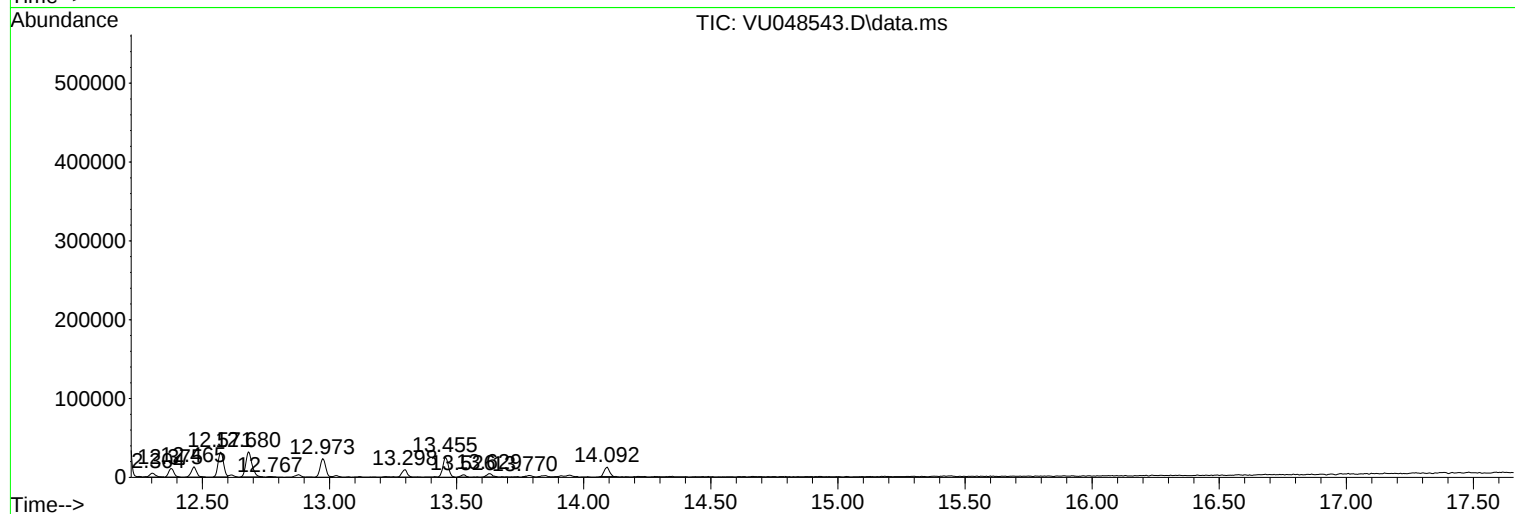
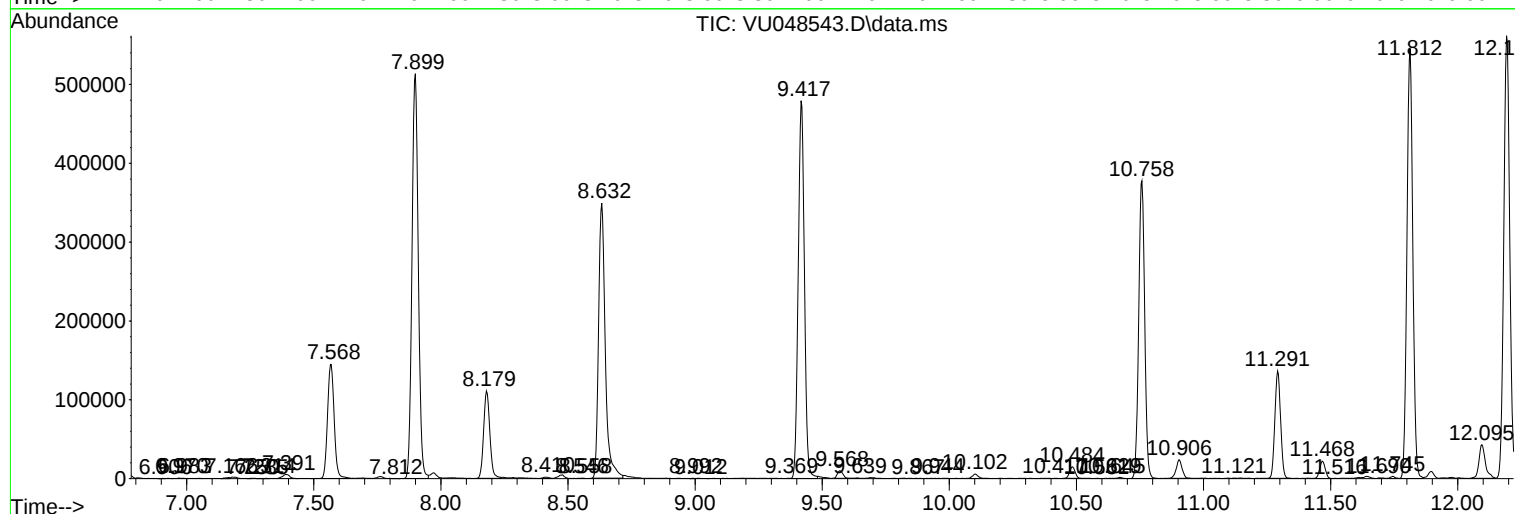
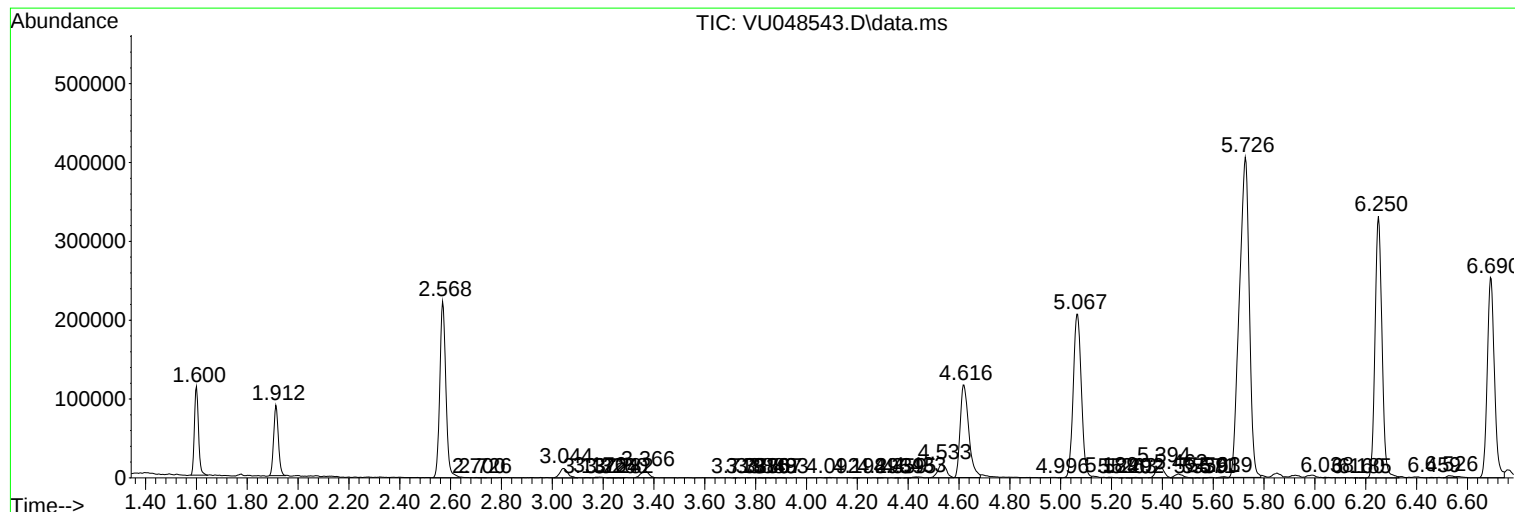
Sum of corrected areas: 9571225

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Instrument :
MSVOA_U
ClientSampleId :
EXLE1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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EXLE1

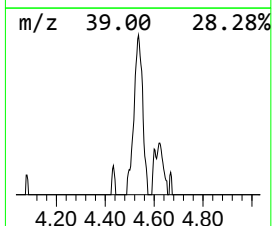
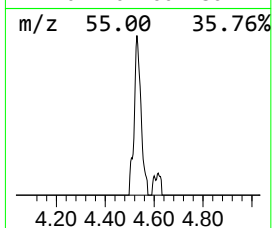
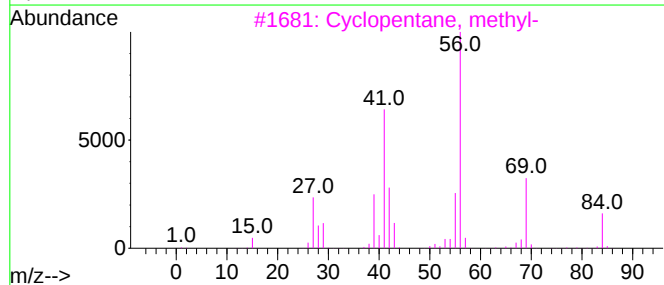
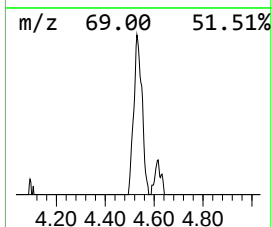
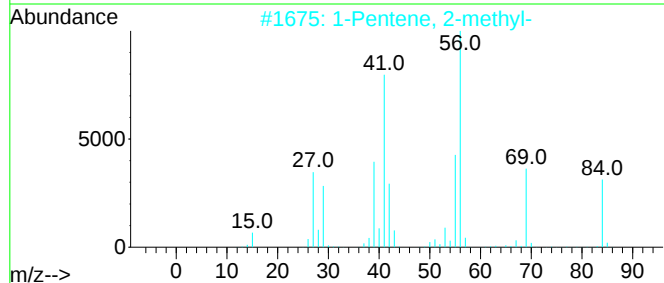
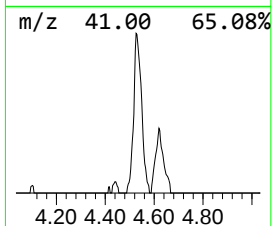
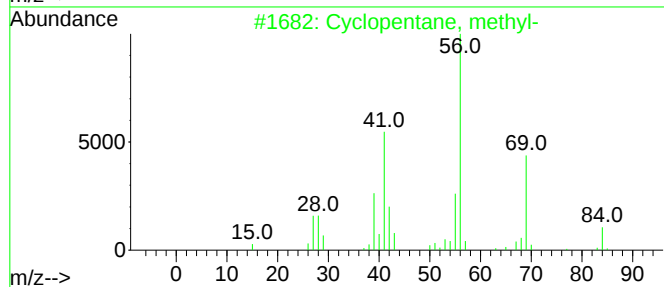
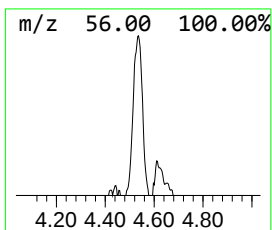
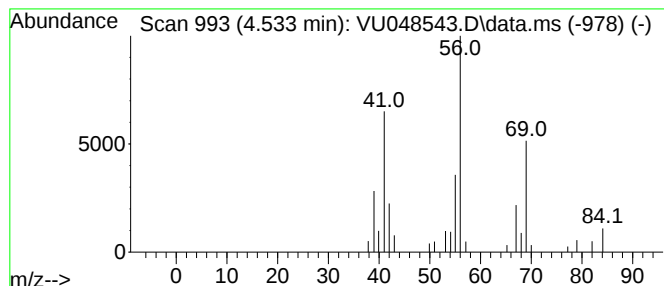
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Cyclic4.533 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.533	3.15 ug/L	39877	1,4-Difluorobenzene	6.250

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	81
2		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	53
3		Cyclopentane, methyl-	84	C6H12	000096-37-7	53
4		Cyclobutane, ethyl-	84	C6H12	004806-61-5	50
5		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	50



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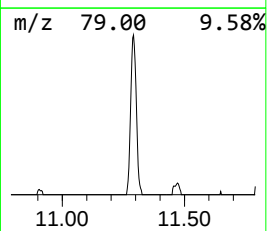
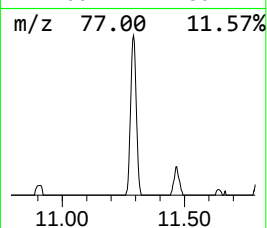
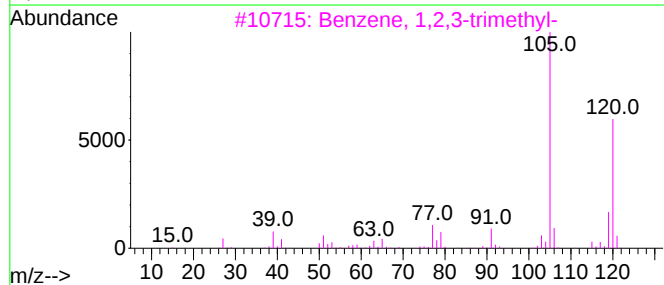
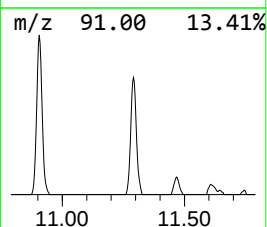
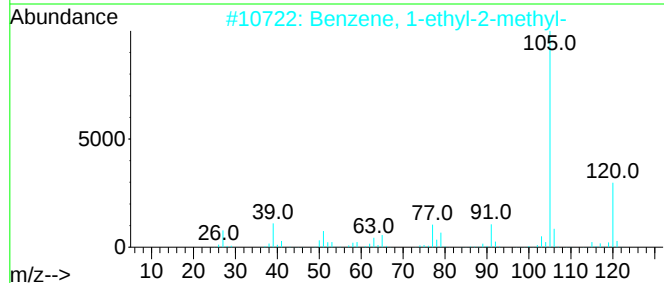
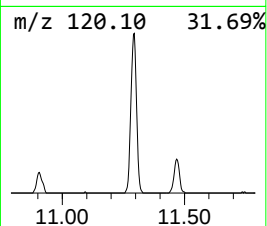
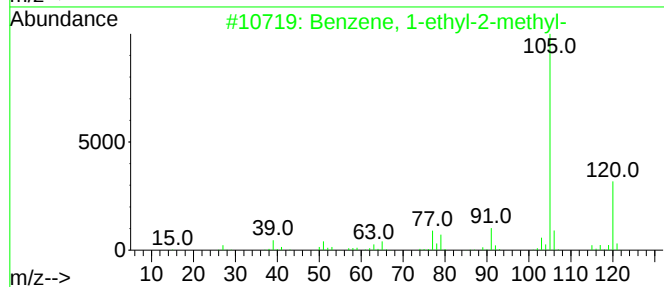
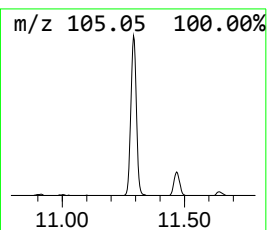
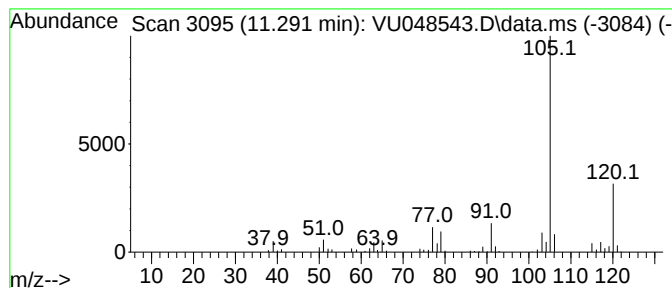
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.291	12.39 ug/L	214303	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Mesitylene	120	C9H12	000108-67-8	91



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ClientSampleId :
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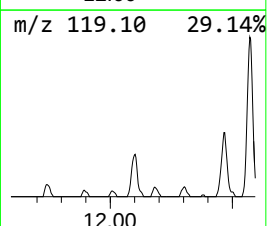
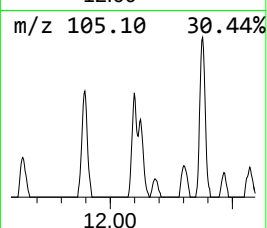
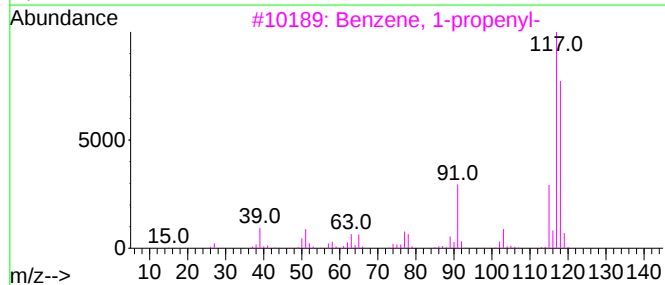
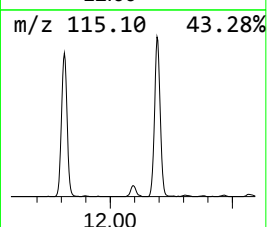
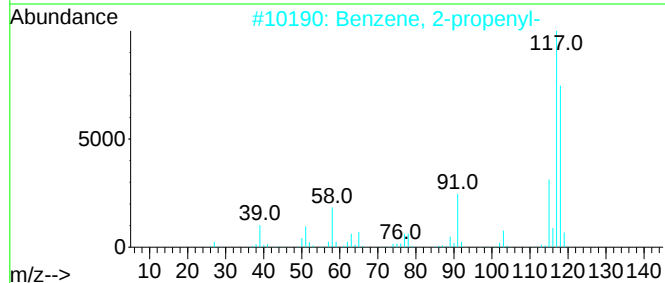
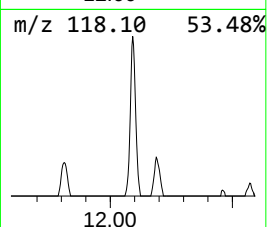
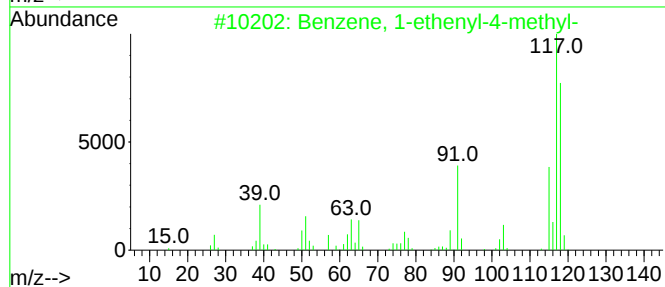
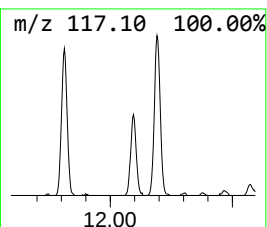
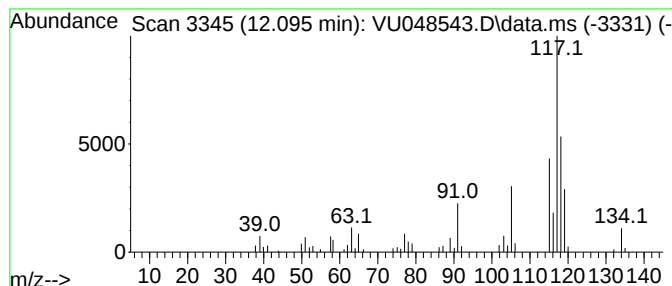
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Benzene, 1-ethenyl-4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.095	4.33 ug/L	74877	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	78
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	60
3			Benzene, 1-propenyl-	118	C9H10	000637-50-3	60
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	60
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	118	C9H10	055337-80-9	60



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051222\
Data File : VU048543.D
Acq On : 12 May 2022 15:49
Operator : SY/MD
Sample : N2801-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXLE1

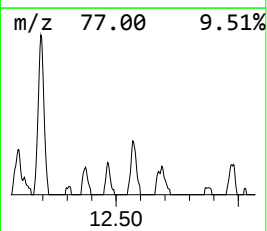
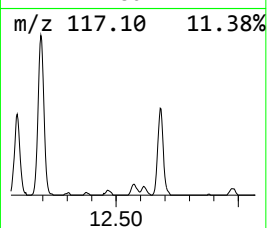
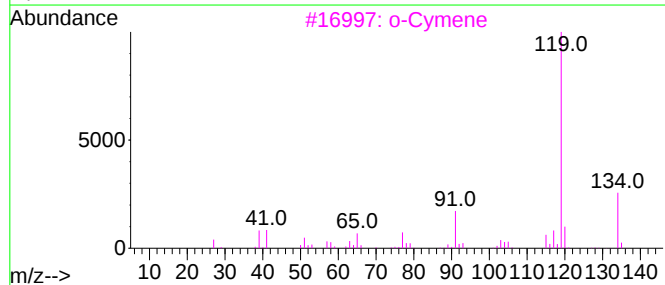
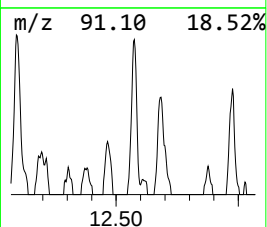
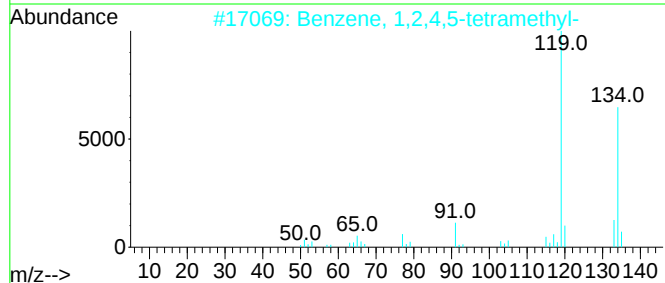
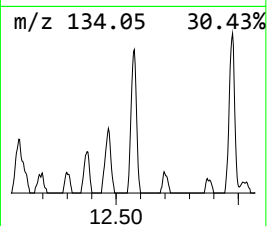
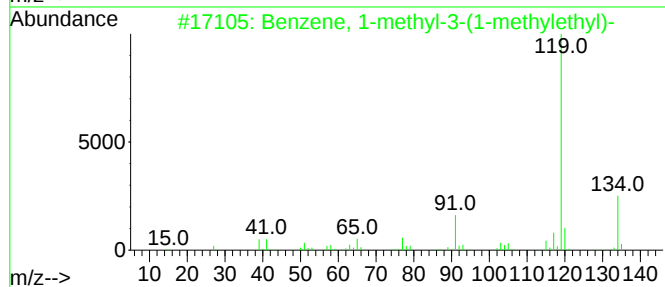
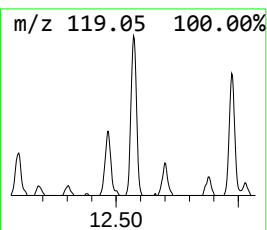
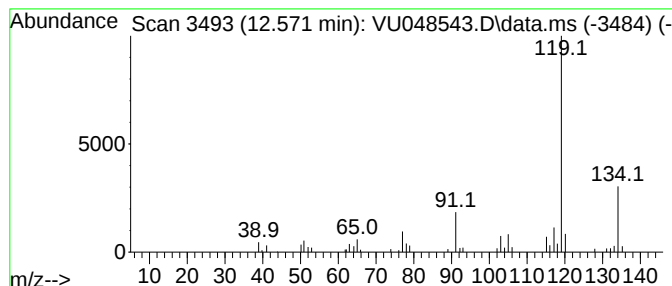
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Quant Title : VOC Analysis

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

Peak Number 5 Benzene, 1-methyl-3-(1-meth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.571	2.69 ug/L	46509	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	91
2			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	91
3			o-Cymene	134	C10H14	000527-84-4	91
4			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	91
5			p-Cymene	134	C10H14	000099-87-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051222\
Data File : VU048543.D
Acq On : 12 May 2022 15:49
Operator : SY/MD
Sample : N2801-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXLE1

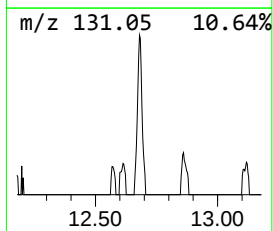
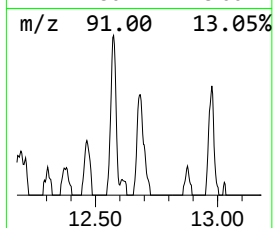
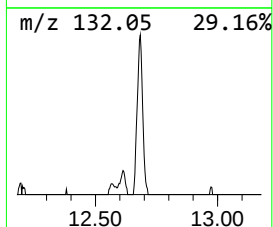
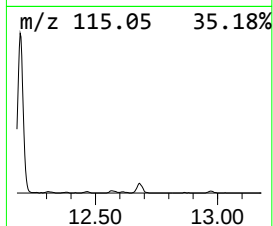
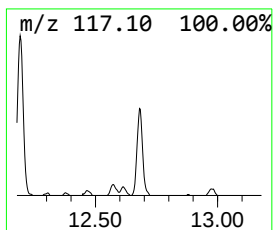
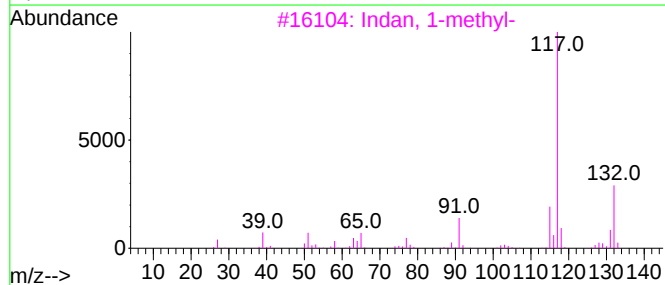
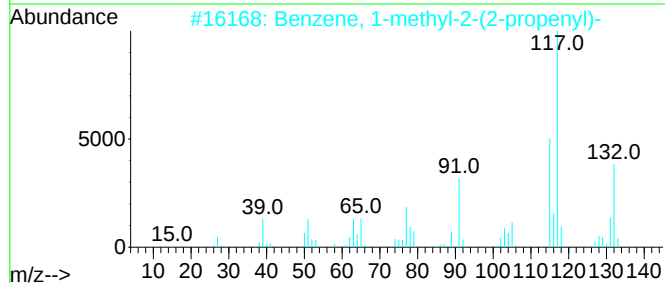
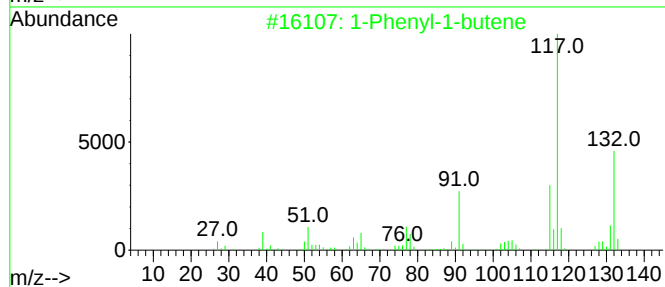
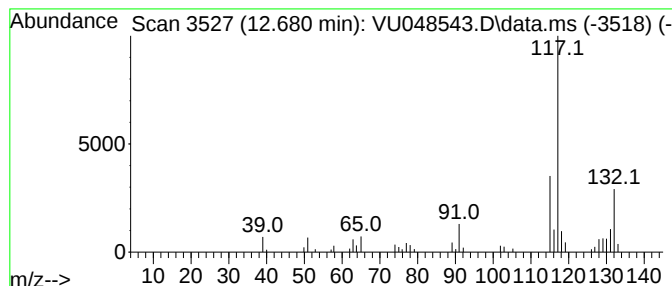
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Quant Title : VOC Analysis

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

Peak Number 6 1-Phenyl-1-butene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	3.12 ug/L	53915	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenyl-1-butene	132	C10H12	000824-90-8	91
2			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	91
3			Indan, 1-methyl-	132	C10H12	000767-58-8	87
4			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	87
5			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051222\
Data File : VU048543.D
Acq On : 12 May 2022 15:49
Operator : SY/MD
Sample : N2801-08
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXLE1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.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
(DEL) Alkane: C...	4.533	3.1	ug/L	39877	1	6.250	632281	50.0
Benzene, 1-ethy...	11.291	12.4	ug/L	214303	3	11.812	865067	50.0
Benzene, 1-ethe...	12.095	4.3	ug/L	74877	3	11.812	865067	50.0
Benzene, 1-meth...	12.571	2.7	ug/L	46509	3	11.812	865067	50.0
1-Phenyl-1-butene	12.680	3.1	ug/L	53915	3	11.812	865067	50.0