

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092022\
 Data File : VU050861.D
 Acq On : 21 Sep 2022 03:25
 Operator : JC/MD
 Sample : N4650-02 25X
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXYZ7

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\SFAMULM092022WMA.M
 Title : VOC Analysis

Signal : TIC: VU050861.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	73	81	99	rVB2	441830	554479	28.64%	2.734%
2	1.909	169	177	181	rBV	212802	282023	14.56%	1.391%
3	2.565	368	381	398	rBV	389731	648737	33.50%	3.199%
4	2.781	445	448	452	rBV2	891	829	0.04%	0.004%
5	2.832	461	464	468	rBV4	515	374	0.02%	0.002%
6	3.044	519	530	543	rBV2	11413	21005	1.08%	0.104%
7	3.186	559	574	588	rBV	19765	46659	2.41%	0.230%
8	3.353	615	626	639	rBV3	10025	19958	1.03%	0.098%
9	3.478	659	665	670	rBV2	314	369	0.02%	0.002%
10	3.636	708	714	722	rBV	1003	1452	0.07%	0.007%
11	3.867	767	786	812	rBV	340292	805697	41.61%	3.973%
12	4.006	827	829	834	rBV4	445	428	0.02%	0.002%
13	4.260	904	908	913	rVB3	465	382	0.02%	0.002%
14	4.623	1005	1021	1025	rBV	230876	425719	21.99%	2.099%
15	4.899	1104	1107	1109	rBV2	581	330	0.02%	0.002%
16	5.063	1140	1158	1179	rBV	344976	758571	39.18%	3.740%
17	5.202	1198	1201	1204	rBV3	470	391	0.02%	0.002%
18	5.221	1204	1207	1210	rVV3	713	572	0.03%	0.003%
19	5.237	1210	1212	1214	rVV	618	354	0.02%	0.002%
20	5.314	1217	1236	1253	rBV2	54238	123905	6.40%	0.611%
21	5.465	1279	1283	1286	rVB3	575	362	0.02%	0.002%
22	5.507	1291	1296	1298	rBV2	505	383	0.02%	0.002%
23	5.639	1331	1337	1340	rBV2	303	330	0.02%	0.002%
24	5.723	1342	1363	1395	rBV2	709824	1936363	100.00%	9.547%
25	6.047	1462	1464	1468	rVB2	874	664	0.03%	0.003%
26	6.247	1511	1526	1551	rBV	541029	1015444	52.44%	5.007%
27	6.536	1604	1616	1631	rVB7	14685	31254	1.61%	0.154%
28	6.690	1649	1664	1682	rBV	453484	885064	45.71%	4.364%
29	6.912	1729	1733	1737	rBV3	571	453	0.02%	0.002%
30	6.993	1751	1758	1761	rBV3	1371	1787	0.09%	0.009%
31	7.134	1797	1802	1805	rVB3	348	332	0.02%	0.002%
32	7.182	1811	1817	1819	rBV3	1631	1566	0.08%	0.008%
33	7.565	1923	1936	1961	rBV	213871	378828	19.56%	1.868%
34	7.790	2001	2006	2011	rBV5	456	565	0.03%	0.003%
35	7.896	2025	2039	2053	rBV	794705	1369864	70.74%	6.754%
36	7.967	2053	2061	2075	rVB	65375	116854	6.03%	0.576%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092022WMA.M
 Title : VOC Analysis

37	8.099	2096	2102	2104	rBV5	385	350	0.02%	0.002%
38	8.179	2113	2127	2148	rBV	149425	258627	13.36%	1.275%
39	8.304	2161	2166	2169	rBV4	789	639	0.03%	0.003%
40	8.398	2190	2195	2202	rVV3	1982	2533	0.13%	0.012%
41	8.478	2218	2220	2228	rVB3	990	839	0.04%	0.004%
42	8.555	2233	2244	2254	rBV6	2666	4418	0.23%	0.022%
43	8.632	2254	2268	2300	rBV2	596927	1151694	59.48%	5.679%
44	8.861	2336	2339	2342	rBV3	560	381	0.02%	0.002%
45	8.874	2342	2343	2348	rVB3	639	417	0.02%	0.002%
46	8.909	2352	2354	2359	rVB3	576	395	0.02%	0.002%
47	8.935	2359	2362	2365	rBV2	494	344	0.02%	0.002%
48	8.983	2374	2377	2379	rBV2	551	328	0.02%	0.002%
49	9.333	2483	2486	2493	rVB3	542	546	0.03%	0.003%
50	9.417	2498	2512	2543	rBV	761785	1245214	64.31%	6.140%
51	9.568	2548	2559	2575	rVB	174514	278127	14.36%	1.371%
52	9.690	2582	2597	2613	rBV	375846	620382	32.04%	3.059%
53	9.790	2626	2628	2630	rBV2	614	322	0.02%	0.002%
54	10.099	2711	2724	2738	rBV	214553	340377	17.58%	1.678%
55	10.211	2754	2759	2762	rVB3	451	354	0.02%	0.002%
56	10.237	2764	2767	2771	rVB4	538	514	0.03%	0.003%
57	10.414	2819	2822	2826	rBV2	440	337	0.02%	0.002%
58	10.481	2834	2843	2855	rVB2	17740	28578	1.48%	0.141%
59	10.539	2855	2861	2863	rBV3	411	420	0.02%	0.002%
60	10.619	2884	2886	2891	rVB2	483	353	0.02%	0.002%
61	10.668	2891	2901	2911	rBV6	2076	4032	0.21%	0.020%
62	10.755	2914	2928	2947	rBV	649562	1041238	53.77%	5.134%
63	10.835	2951	2953	2960	rVB4	1150	1213	0.06%	0.006%
64	10.902	2962	2974	2988	rBV	61815	97557	5.04%	0.481%
65	10.996	2990	3003	3021	rBV	216833	481065	24.84%	2.372%
66	11.086	3021	3031	3048	rVB	130138	202126	10.44%	0.997%
67	11.201	3064	3067	3069	rBV2	953	579	0.03%	0.003%
68	11.230	3069	3076	3083	rBV4	4307	6995	0.36%	0.034%
69	11.291	3083	3095	3108	rVB	160915	252643	13.05%	1.246%
70	11.372	3117	3120	3125	rVB5	744	670	0.03%	0.003%
71	11.417	3125	3134	3135	rBV4	963	1231	0.06%	0.006%
72	11.465	3137	3149	3169	rBV	699886	1061860	54.84%	5.236%
73	11.642	3201	3204	3214	rVB5	4123	4750	0.25%	0.023%
74	11.690	3214	3219	3224	rBV5	2007	1969	0.10%	0.010%
75	11.742	3226	3235	3243	rBV2	7460	11229	0.58%	0.055%
76	11.809	3243	3256	3271	rBV	709077	1120655	57.87%	5.525%

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77	11.893	3271	3282	3294	rVB	210120	329205	17.00%	1.623%
78	12.092	3332	3344	3362	rVV3	92123	166707	8.61%	0.822%
79	12.192	3362	3375	3395	rVV	770266	1252775	64.70%	6.177%
80	12.375	3424	3432	3445	rVB	7103	11379	0.59%	0.056%
81	12.478	3450	3464	3485	rBV	383566	705441	36.43%	3.478%
82	12.568	3487	3492	3502	rVB	17748	26175	1.35%	0.129%
83	12.680	3520	3527	3545	rVB7	8272	17387	0.90%	0.086%
84	12.877	3580	3588	3597	rBV5	5827	8685	0.45%	0.043%
85	12.973	3603	3618	3626	rBV5	9095	14987	0.77%	0.074%
86	13.025	3626	3634	3645	rVB2	14633	21701	1.12%	0.107%
87	13.201	3686	3689	3691	rBV2	503	348	0.02%	0.002%
88	13.217	3691	3694	3697	rVV3	567	410	0.02%	0.002%
89	13.291	3710	3717	3725	rVB8	4101	5695	0.29%	0.028%
90	13.343	3731	3733	3736	rBV	434	326	0.02%	0.002%
91	13.449	3758	3766	3776	rVB6	14445	23719	1.22%	0.117%
92	13.581	3804	3807	3811	rVB2	602	454	0.02%	0.002%
93	13.623	3811	3820	3833	rBV9	3839	6601	0.34%	0.033%
94	13.674	3833	3836	3839	rBV3	466	417	0.02%	0.002%
95	13.899	3900	3906	3908	rBV3	622	683	0.04%	0.003%
96	14.089	3953	3965	3977	rBV3	16510	28068	1.45%	0.138%
97	14.459	4077	4080	4083	rBV	657	336	0.02%	0.002%
98	14.529	4099	4102	4104	rBV2	489	344	0.02%	0.002%
99	14.809	4186	4189	4193	rVB3	566	359	0.02%	0.002%
100	14.835	4193	4197	4201	rBV4	770	769	0.04%	0.004%

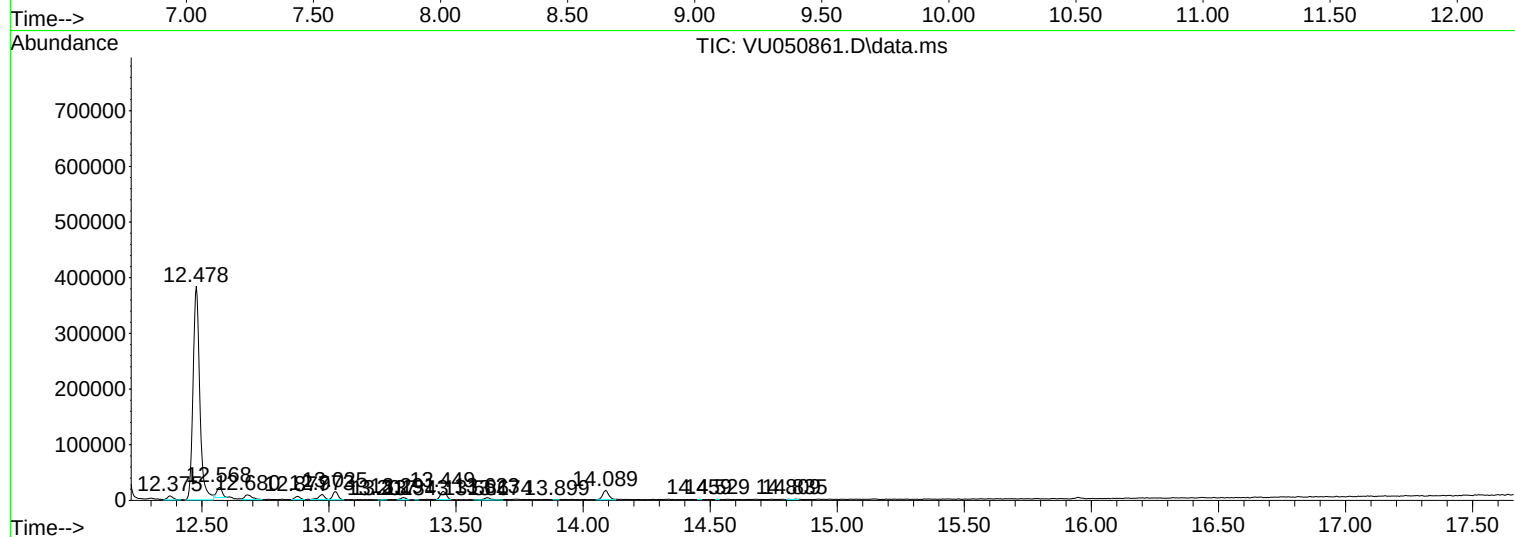
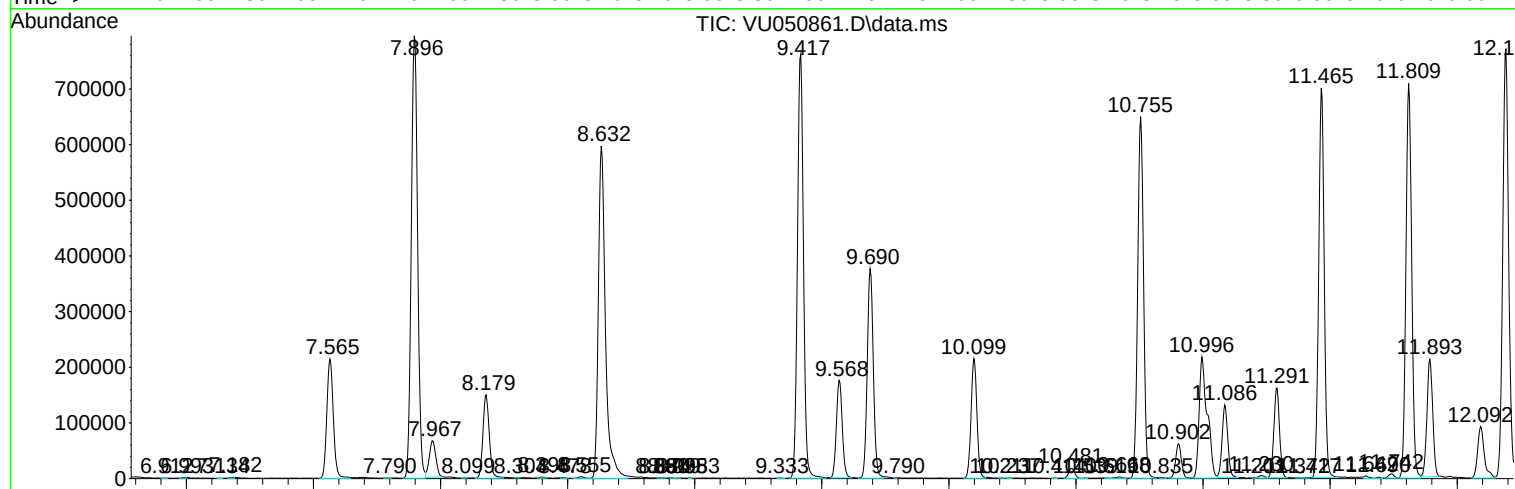
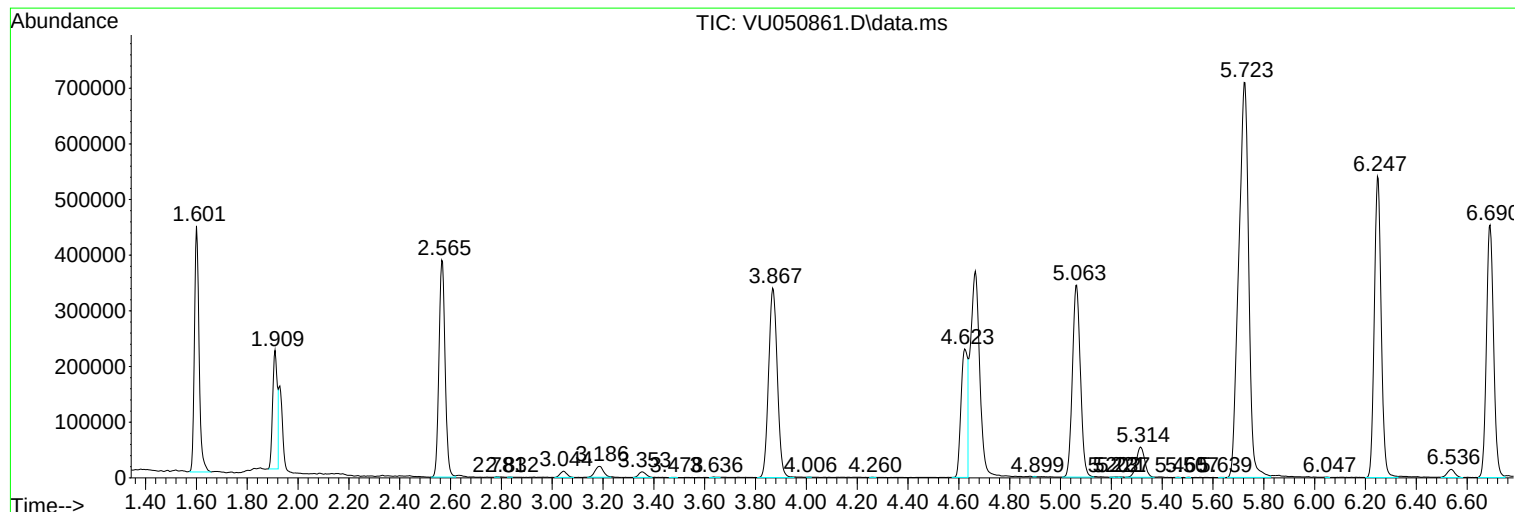
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MSVOA_U
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092022WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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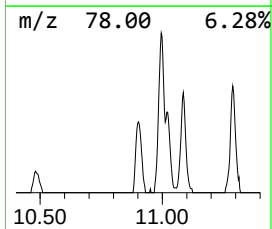
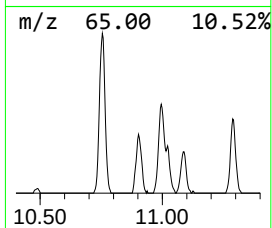
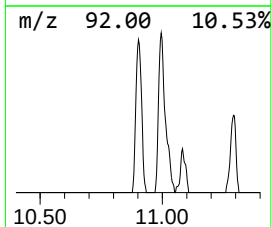
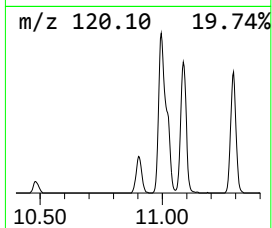
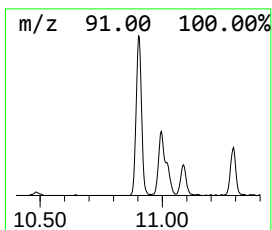
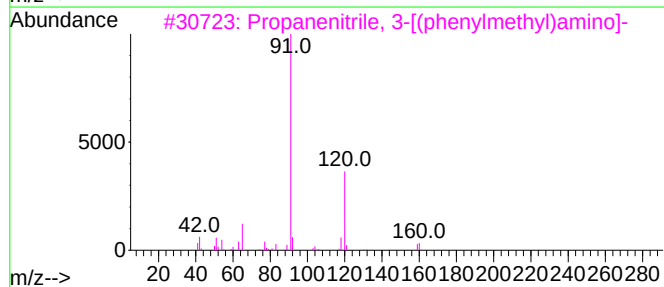
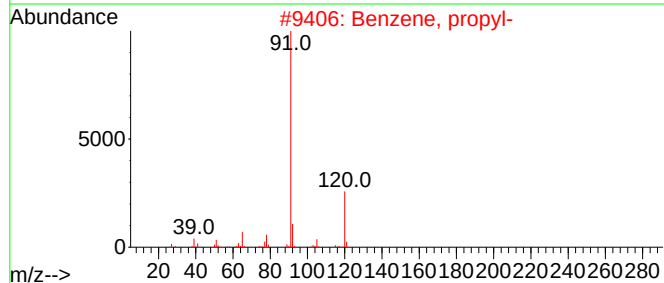
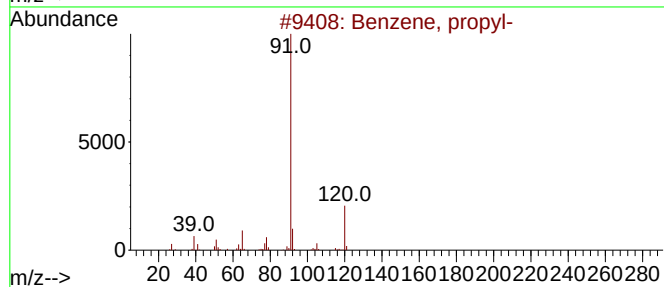
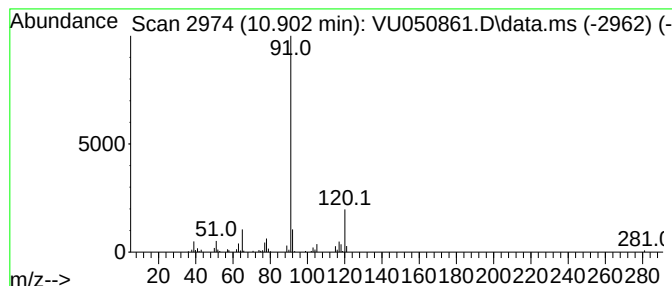
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092022WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, propyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.902	4.35 ug/L	97557	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, propyl-	120	C9H12	000103-65-1	81
2			Benzene, propyl-	120	C9H12	000103-65-1	74
3			Propanenitrile, 3-[(phenylmethyl)amino]-	160	C10H12N2	000706-03-6	64
4			Benzene, propyl-	120	C9H12	000103-65-1	62
5			1,2-Ethanediamine, N-(phenylmeth)amino	150	C9H14N2	004152-09-4	59



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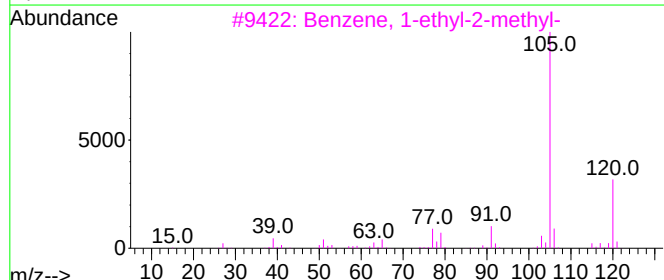
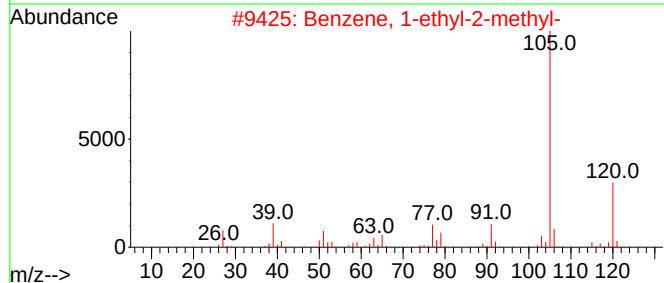
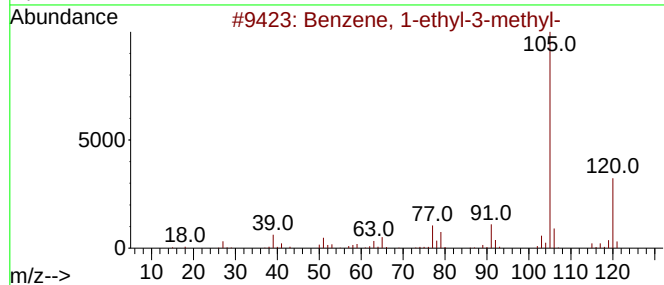
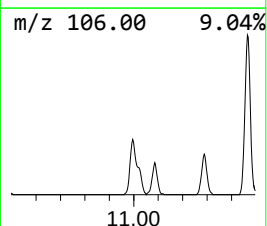
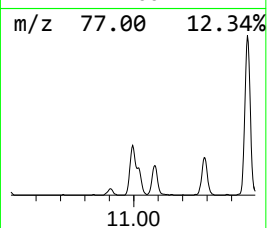
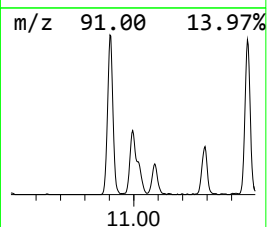
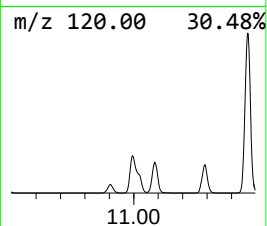
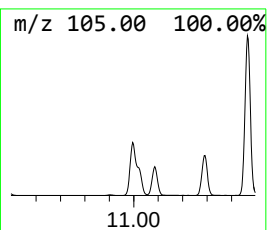
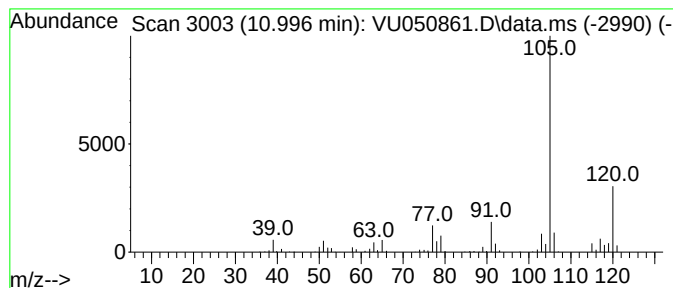
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092022WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.996	21.46 ug/L	481065	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



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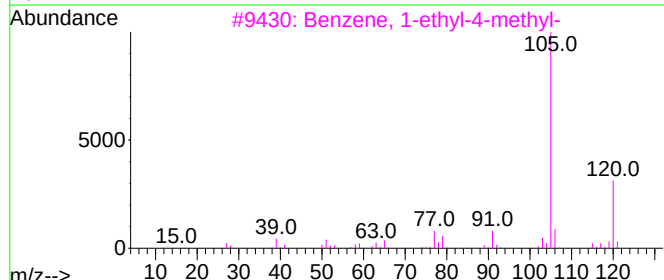
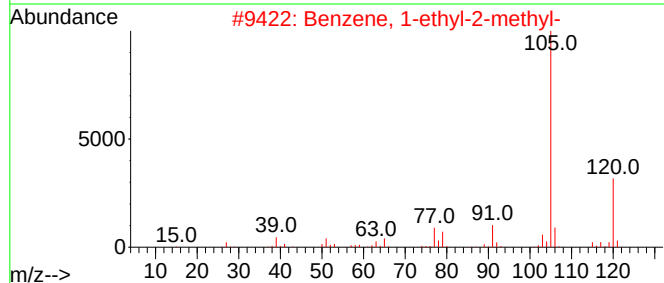
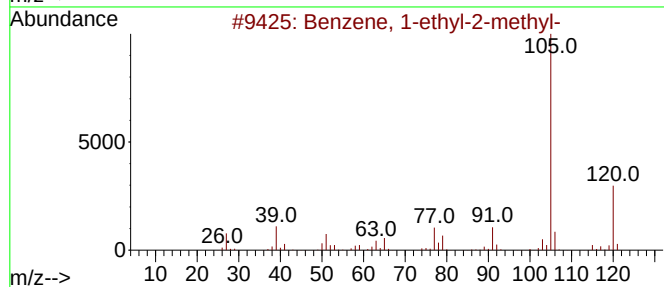
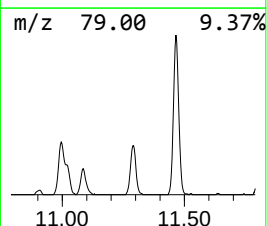
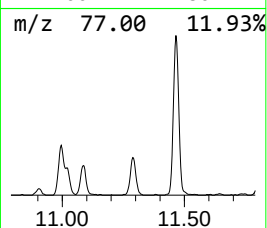
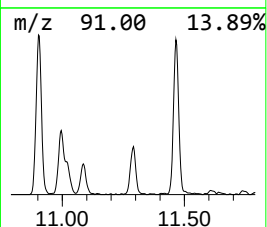
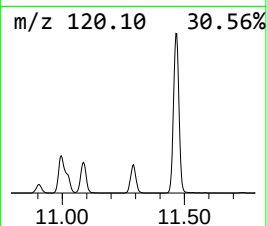
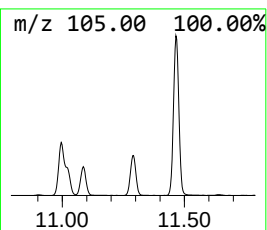
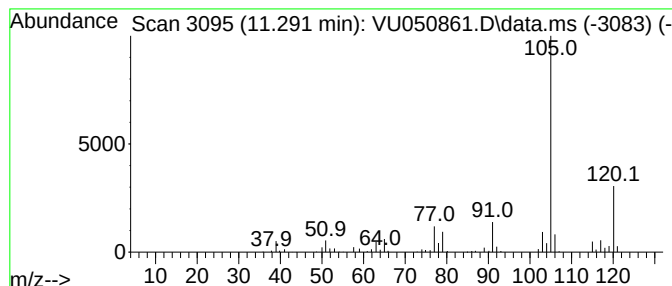
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.291	11.27 ug/L	252643	1,4-Dichlorobenzene-d4	11.809

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092022\
Data File : VU050861.D
Acq On : 21 Sep 2022 03:25
Operator : JC/MD
Sample : N4650-02 25X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXYZ7

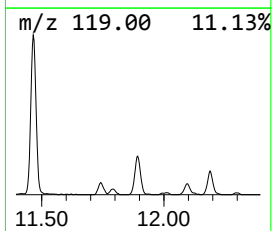
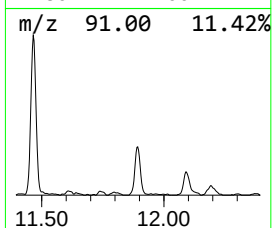
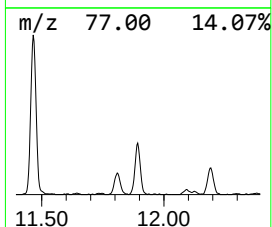
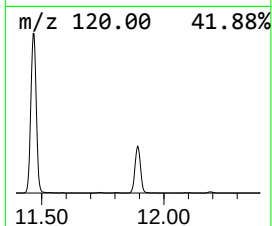
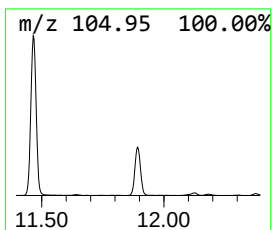
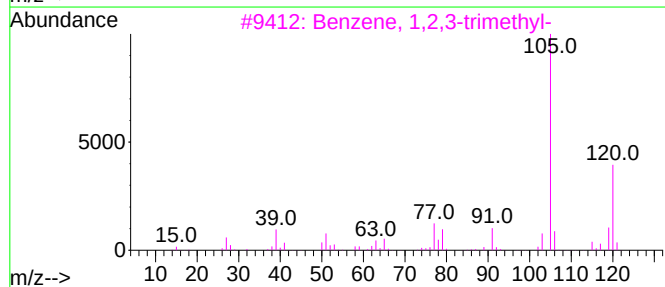
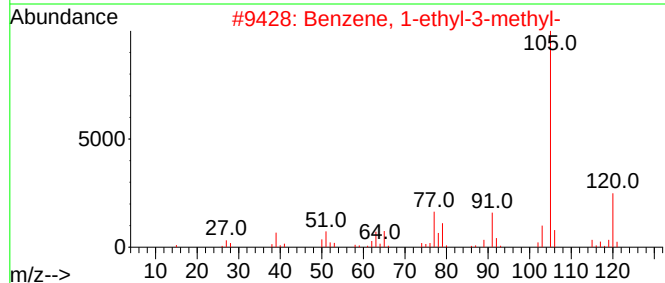
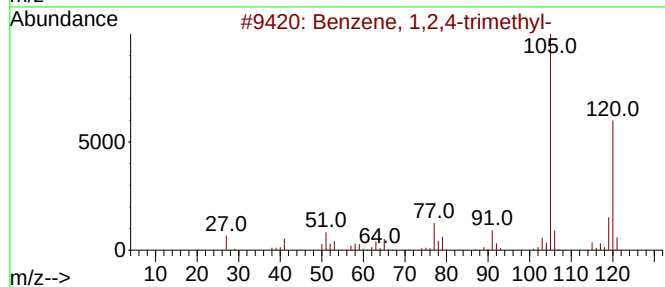
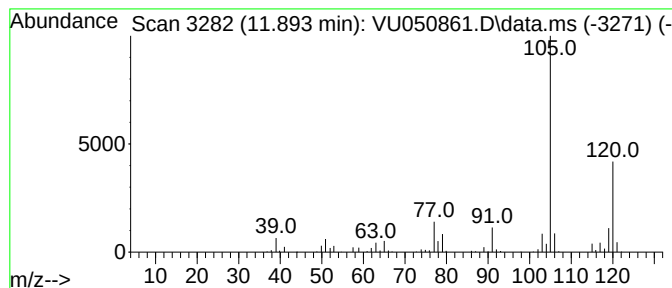
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.893	14.69 ug/L	329205	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092022\
Data File : VU050861.D
Acq On : 21 Sep 2022 03:25
Operator : JC/MD
Sample : N4650-02 25X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXYZ7

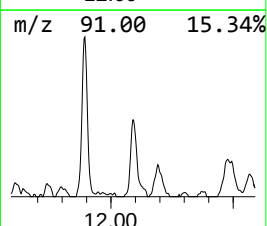
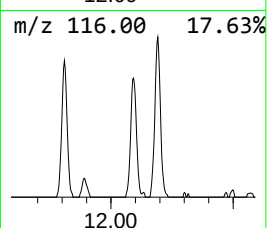
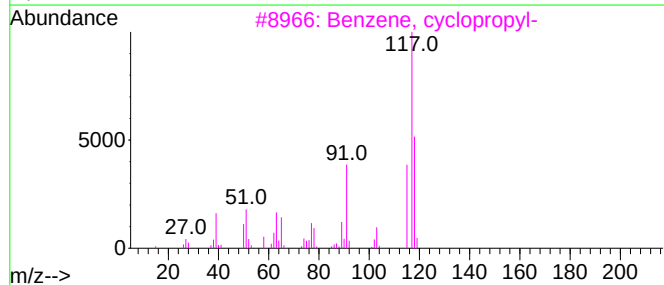
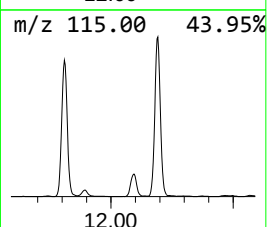
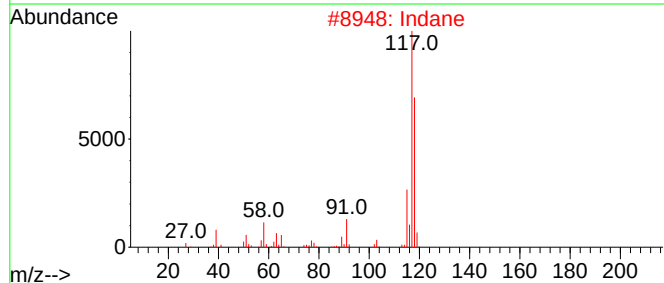
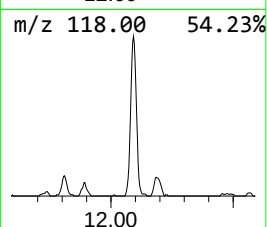
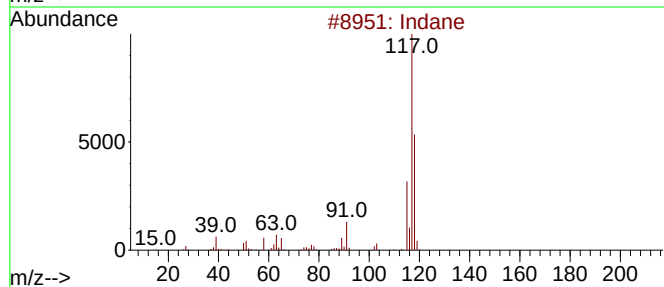
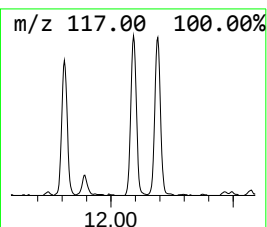
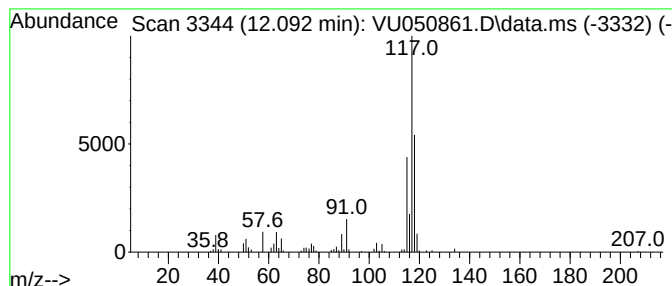
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Indane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.092	7.44 ug/L	166707	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane			118	C9H10	000496-11-7	93
2	Indane			118	C9H10	000496-11-7	93
3	Benzene, cyclopropyl-			118	C9H10	000873-49-4	70
4	Benzene, 1-ethenyl-4-methyl-			118	C9H10	000622-97-9	68
5	3-Bromo-1-phenyl-1-propene			196	C9H9Br	004392-24-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092022\
Data File : VU050861.D
Acq On : 21 Sep 2022 03:25
Operator : JC/MD
Sample : N4650-02 25X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXYZ7

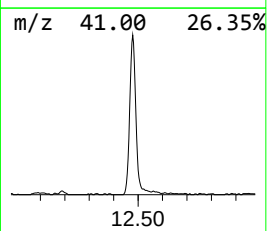
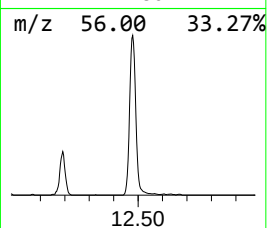
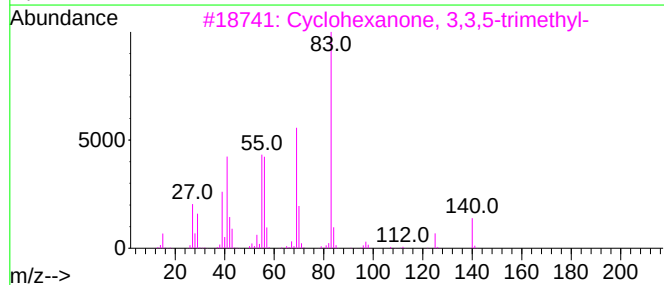
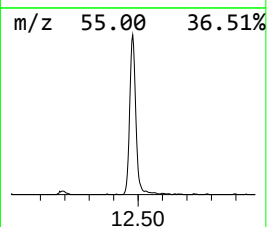
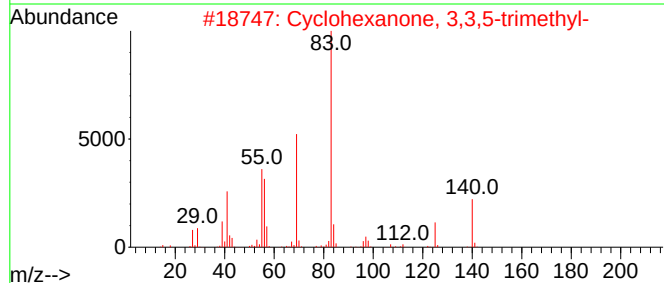
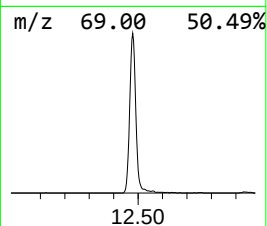
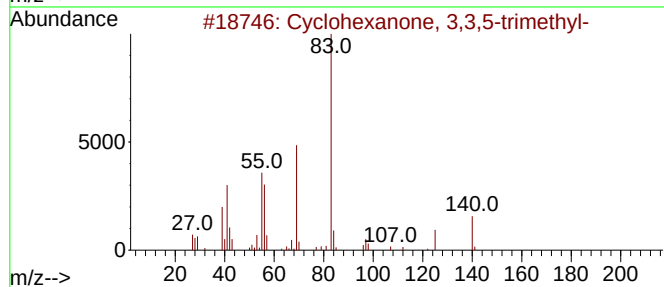
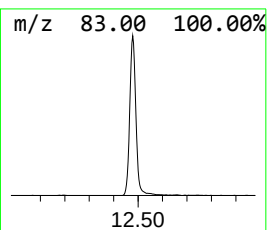
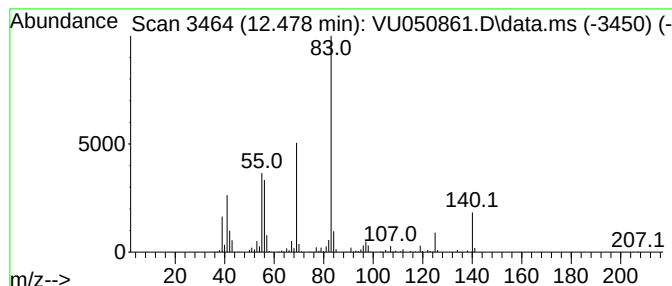
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092022WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Cyclohexanone, 3,3,5-trimet... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.478	31.47 ug/L	705441	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	97
2			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	95
3			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	91
4			1-Methyl-1H-1,2,4-triazole	83	C3H5N3	006086-21-1	53
5			1H-1,2,4-Triazole, 3-(2-methylpr...	125	C6H11N3	040515-29-5	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092022\
Data File : VU050861.D
Acq On : 21 Sep 2022 03:25
Operator : JC/MD
Sample : N4650-02 25X
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EXYZ7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092022WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, propyl-	10.902	4.3	ug/L	97557	3	11.809	1120660	50.0
Benzene, 1-ethy...	10.996	21.5	ug/L	481065	3	11.809	1120660	50.0
Benzene, 1-ethy...	11.291	11.3	ug/L	252643	3	11.809	1120660	50.0
Benzene, 1,2,3-...	11.893	14.7	ug/L	329205	3	11.809	1120660	50.0
Indane	12.092	7.4	ug/L	166707	3	11.809	1120660	50.0
Cyclohexanone, ...	12.478	31.5	ug/L	705441	3	11.809	1120660	50.0