

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121321\
 Data File : VU046325.D
 Acq On : 13 Dec 2021 18:58
 Operator : SY/MD
 Sample : M4983-21
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW5S2

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\SFAMULM112921WMA.M
 Title : VOC Analysis

Signal : TIC: VU046325.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	75	81	92	rVB	77760	85175	15.73%	1.677%
2	1.919	173	180	184	rBV	56517	75409	13.93%	1.485%
3	2.218	270	273	275	rBV2	411	284	0.05%	0.006%
4	2.305	298	300	302	rBV3	516	295	0.05%	0.006%
5	2.440	339	342	344	rBV	511	366	0.07%	0.007%
6	2.572	371	383	405	rBV	115362	192306	35.51%	3.787%
7	2.787	446	450	452	rBV2	509	358	0.07%	0.007%
8	3.105	546	549	554	rVB	588	439	0.08%	0.009%
9	3.131	554	557	560	rBV	421	343	0.06%	0.007%
10	3.170	566	569	570	rBV2	396	227	0.04%	0.004%
11	3.359	622	628	642	rBV5	1028	1917	0.35%	0.038%
12	3.456	653	658	661	rBV	483	514	0.09%	0.010%
13	3.555	686	689	692	rBV2	290	191	0.04%	0.004%
14	3.700	730	734	736	rBV	497	379	0.07%	0.007%
15	3.797	761	764	766	rBV2	310	224	0.04%	0.004%
16	3.877	776	789	809	rVB	37343	87078	16.08%	1.715%
17	4.054	842	844	848	rBV	391	268	0.05%	0.005%
18	4.080	848	852	854	rBV	359	262	0.05%	0.005%
19	4.179	879	883	886	rBV	339	293	0.05%	0.006%
20	4.256	903	907	910	rBV2	395	301	0.06%	0.006%
21	4.424	953	959	962	rBV2	322	381	0.07%	0.008%
22	4.440	962	964	967	rVV	299	191	0.04%	0.004%
23	4.504	981	984	988	rBV	268	243	0.04%	0.005%
24	4.642	1010	1027	1065	rBV2	43535	139410	25.74%	2.745%
25	4.957	1117	1125	1130	rBV2	406	664	0.12%	0.013%
26	5.067	1144	1159	1181	rBV	95406	220489	40.72%	4.342%
27	5.195	1195	1199	1201	rBV2	269	188	0.03%	0.004%
28	5.321	1224	1238	1252	rBV2	22185	47068	8.69%	0.927%
29	5.478	1284	1287	1290	rBV2	487	369	0.07%	0.007%
30	5.588	1317	1321	1326	rBV2	337	346	0.06%	0.007%
31	5.649	1337	1340	1342	rBV	395	246	0.05%	0.005%
32	5.729	1342	1365	1389	rVV3	199664	541533	100.00%	10.665%
33	5.941	1428	1431	1433	rBV2	286	179	0.03%	0.004%
34	6.253	1512	1528	1553	rBV	176544	339189	62.63%	6.680%
35	6.440	1583	1586	1588	rBV	602	411	0.08%	0.008%
36	6.475	1594	1597	1599	rBV	488	324	0.06%	0.006%

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 Title : VOC Analysis

37	6.536	1608	1616	1625	rBV9	2224	3973	0.73%	0.078%
38	6.694	1652	1665	1683	rBV	124110	241482	44.59%	4.756%
39	6.809	1696	1701	1706	rBV2	558	689	0.13%	0.014%
40	7.166	1809	1812	1816	rBV	406	363	0.07%	0.007%
41	7.311	1854	1857	1860	rBV	207	176	0.03%	0.003%
42	7.337	1862	1865	1868	rVB	436	264	0.05%	0.005%
43	7.568	1925	1937	1953	rVV	66054	115401	21.31%	2.273%
44	7.658	1963	1965	1969	rVB	374	191	0.04%	0.004%
45	7.813	2010	2013	2015	rBV	285	195	0.04%	0.004%
46	7.899	2028	2040	2058	rBV	238412	405984	74.97%	7.995%
47	8.182	2117	2128	2142	rBV	47694	78449	14.49%	1.545%
48	8.475	2212	2219	2226	rVB3	3887	5372	0.99%	0.106%
49	8.555	2238	2244	2254	rVB4	3566	5686	1.05%	0.112%
50	8.636	2257	2269	2301	rVV	153954	274800	50.74%	5.412%
51	8.809	2321	2323	2329	rVB3	458	372	0.07%	0.007%
52	8.867	2334	2341	2348	rVB3	2128	2933	0.54%	0.058%
53	8.925	2353	2359	2360	rBV2	839	769	0.14%	0.015%
54	9.060	2396	2401	2405	rBV2	438	475	0.09%	0.009%
55	9.099	2410	2413	2417	rVV	449	349	0.06%	0.007%
56	9.243	2454	2458	2459	rBV	439	328	0.06%	0.006%
57	9.362	2493	2495	2498	rBV	374	215	0.04%	0.004%
58	9.420	2500	2513	2535	rVV	276602	461197	85.17%	9.082%
59	9.568	2552	2559	2570	rVB2	3834	5924	1.09%	0.117%
60	9.780	2620	2625	2628	rBV2	450	480	0.09%	0.009%
61	9.838	2640	2643	2646	rVB	608	423	0.08%	0.008%
62	9.867	2646	2652	2655	rBV	595	639	0.12%	0.013%
63	9.954	2676	2679	2684	rBV	297	282	0.05%	0.006%
64	10.034	2698	2704	2709	rBV3	722	1038	0.19%	0.020%
65	10.134	2731	2735	2739	rBV2	422	478	0.09%	0.009%
66	10.272	2771	2778	2788	rVB5	4231	6077	1.12%	0.120%
67	10.362	2800	2806	2810	rBV5	943	1198	0.22%	0.024%
68	10.411	2818	2821	2825	rVB2	400	311	0.06%	0.006%
69	10.446	2825	2832	2836	rBV	370	575	0.11%	0.011%
70	10.484	2838	2844	2854	rVB4	3337	4939	0.91%	0.097%
71	10.671	2899	2902	2907	rBV3	1049	1100	0.20%	0.022%
72	10.758	2917	2929	2943	rBV	190276	299834	55.37%	5.905%
73	10.906	2961	2975	2989	rBV2	17284	30172	5.57%	0.594%
74	10.999	2995	3004	3009	rBV4	2717	3568	0.66%	0.070%
75	11.089	3022	3032	3044	rBV	24186	36942	6.82%	0.728%
76	11.208	3066	3069	3072	rBV	491	306	0.06%	0.006%

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77	11.295	3087	3096	3113	rVB2	26553	41316	7.63%	0.814%
78	11.417	3127	3134	3140	rVB	790	937	0.17%	0.018%
79	11.468	3140	3150	3162	rBV	73058	113700	21.00%	2.239%
80	11.578	3181	3184	3185	rBV	388	243	0.04%	0.005%
81	11.613	3188	3195	3198	rBV4	2760	3791	0.70%	0.075%
82	11.745	3228	3236	3244	rBV	8396	11090	2.05%	0.218%
83	11.812	3245	3257	3272	rVV	337186	519489	95.93%	10.230%
84	11.896	3275	3283	3294	rVB	17355	25181	4.65%	0.496%
85	11.970	3301	3306	3307	rBV2	1176	983	0.18%	0.019%
86	12.060	3328	3334	3336	rBV5	1639	1758	0.32%	0.035%
87	12.099	3339	3346	3350	rBV3	15317	20915	3.86%	0.412%
88	12.195	3363	3376	3393	rVB	291333	482068	89.02%	9.493%
89	12.378	3424	3433	3443	rBV	11172	16118	2.98%	0.317%
90	12.465	3452	3460	3465	rBV	8581	12958	2.39%	0.255%
91	12.574	3486	3494	3501	rBV	12798	17376	3.21%	0.342%
92	12.652	3514	3518	3519	rBV	319	216	0.04%	0.004%
93	12.687	3520	3529	3530	rBV2	7441	8843	1.63%	0.174%
94	12.771	3547	3555	3563	rBV3	2208	3560	0.66%	0.070%
95	12.938	3603	3607	3608	rBV	703	508	0.09%	0.010%
96	13.025	3627	3634	3647	rVB2	9543	14870	2.75%	0.293%
97	13.452	3758	3767	3779	rVB4	12689	21690	4.01%	0.427%
98	13.623	3816	3820	3829	rVB4	5605	7367	1.36%	0.145%
99	14.086	3957	3964	3983	rVB	12977	20204	3.73%	0.398%
100	15.015	4250	4253	4260	rBV3	758	897	0.17%	0.018%

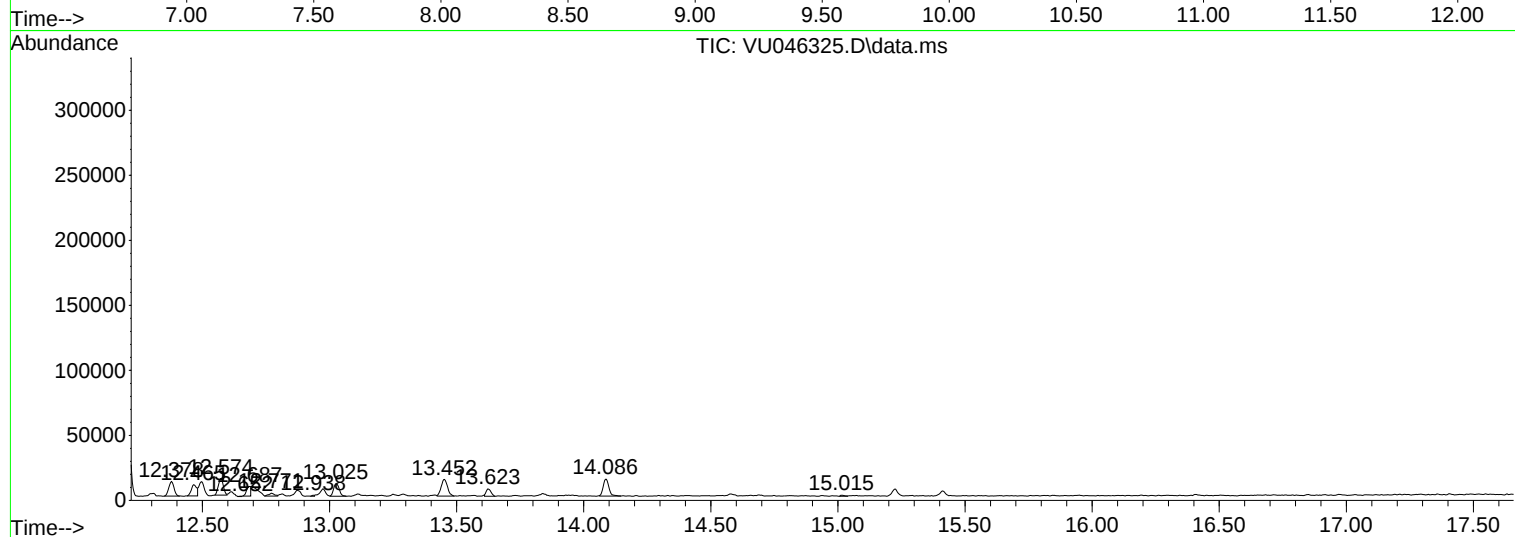
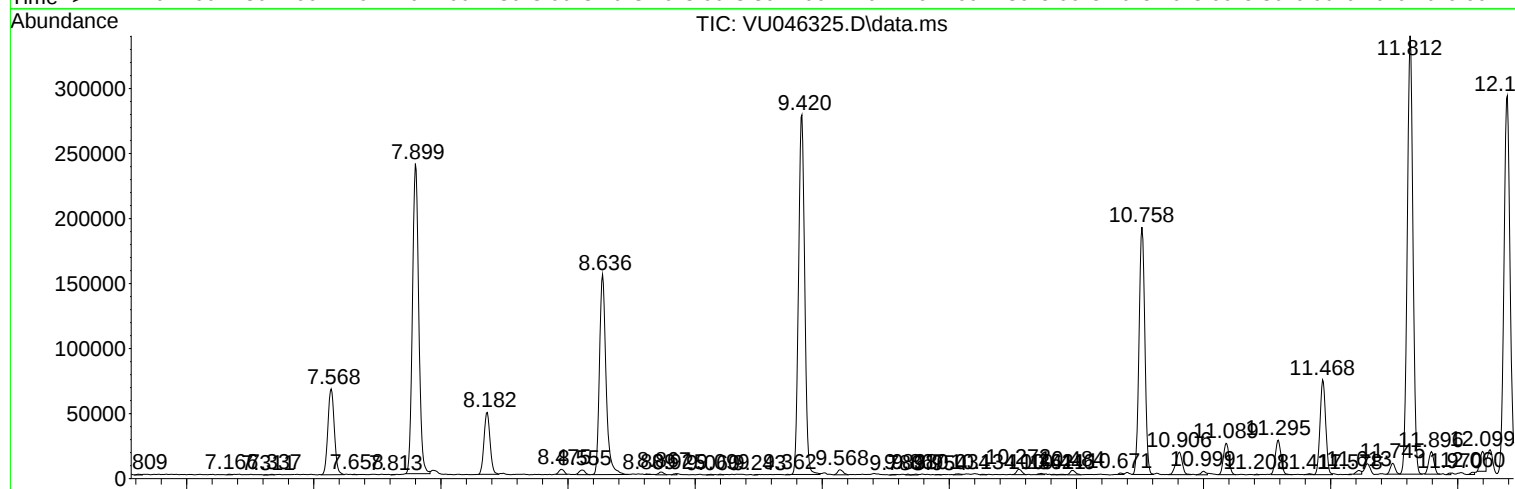
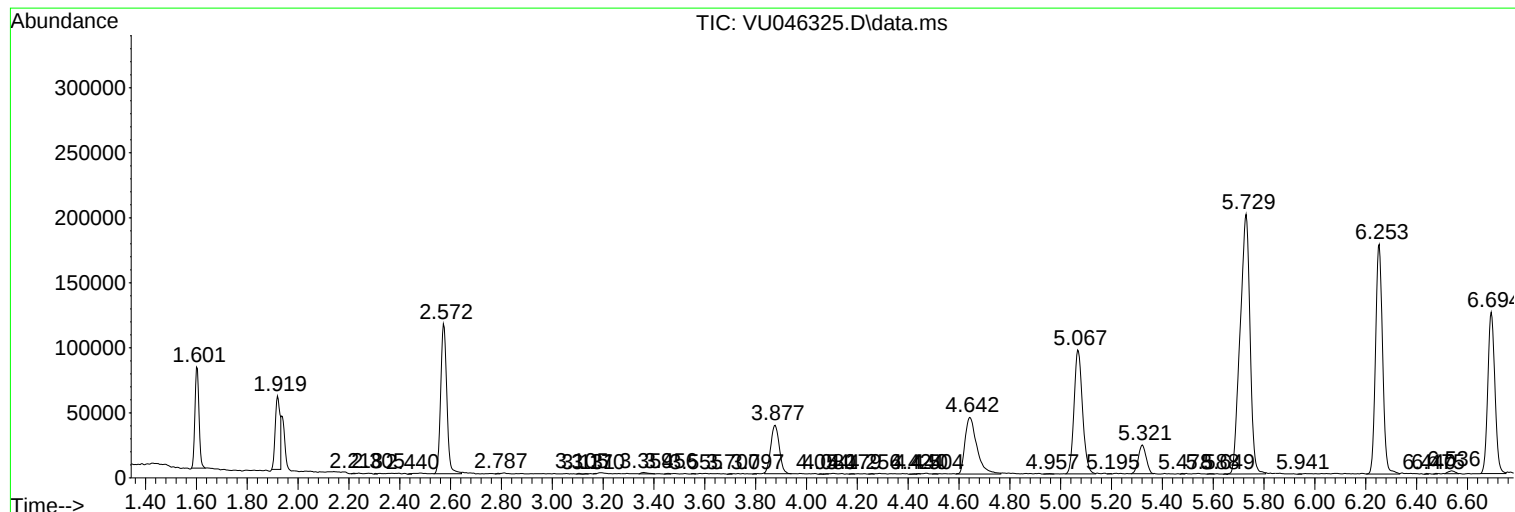
Sum of corrected areas: 5077887

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Quant Title : VOC Analysis

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



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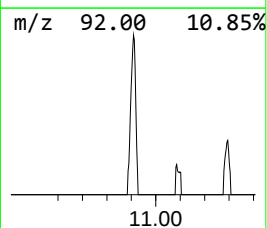
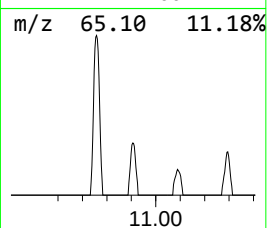
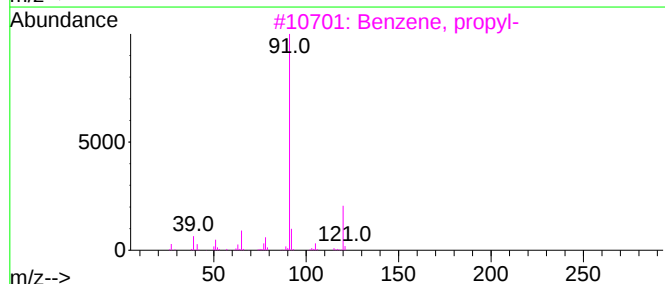
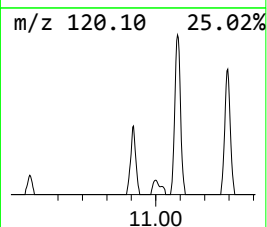
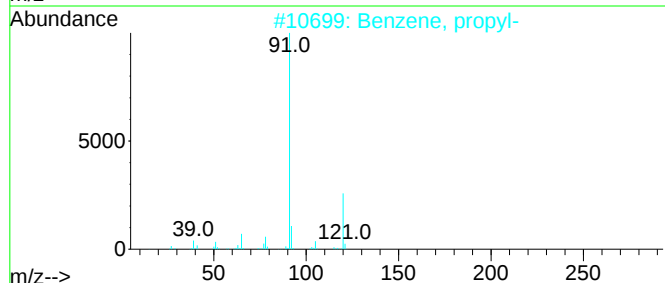
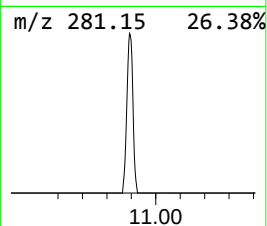
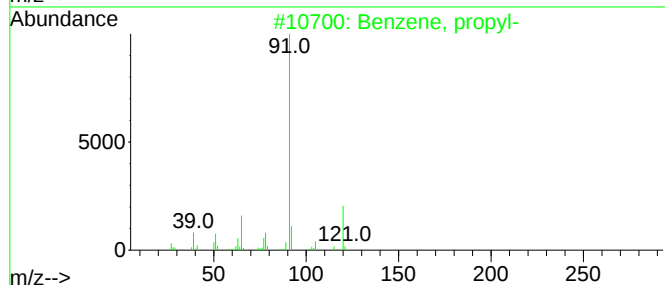
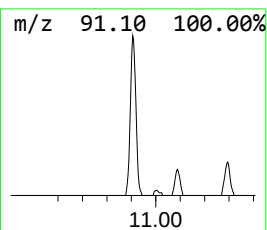
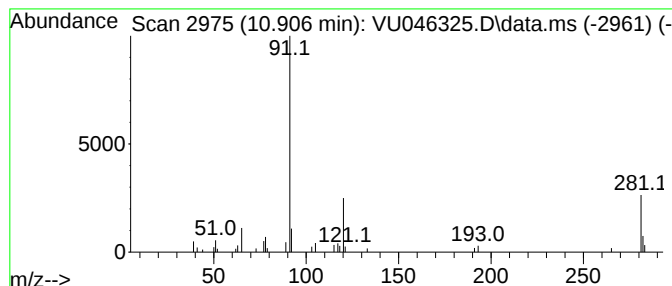
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Benzene, propyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.906	2.90 ug/L	30172	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, propyl-	120	C9H12	000103-65-1	64
2			Benzene, propyl-	120	C9H12	000103-65-1	60
3			Benzene, propyl-	120	C9H12	000103-65-1	60
4			Benzene, propyl-	120	C9H12	000103-65-1	60
5			Acetamide, 2-phenyl-N-benzyl-N-b...	281	C19H23NO	1010446-79-6	59



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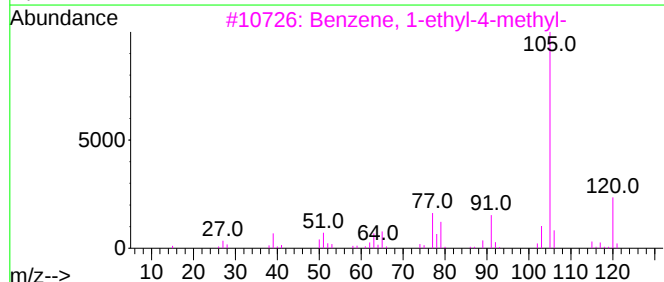
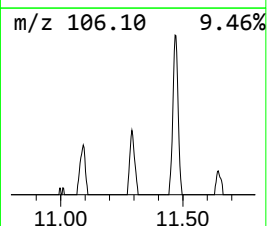
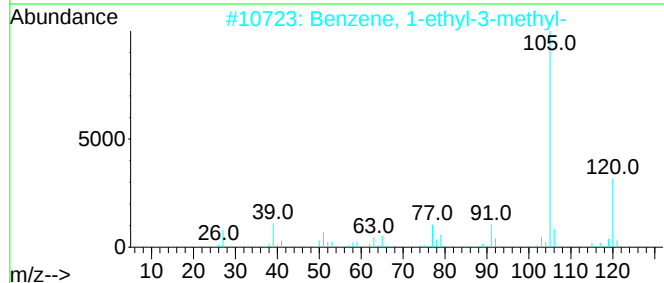
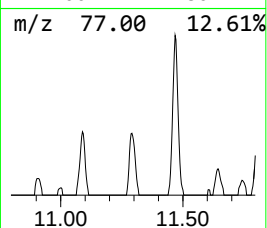
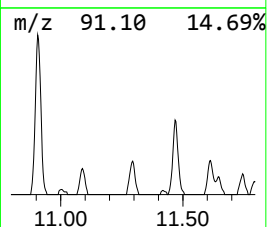
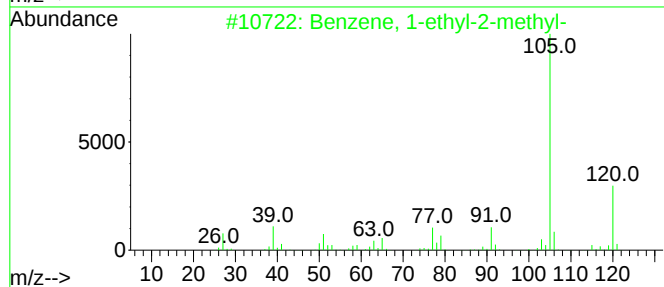
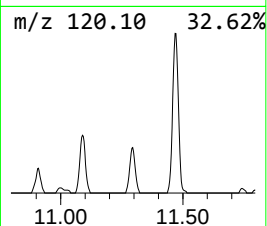
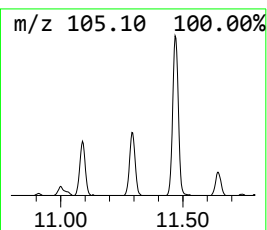
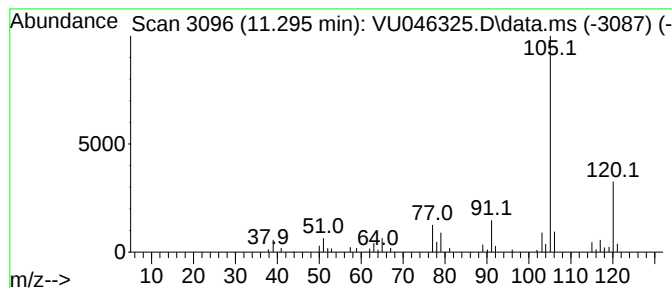
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Quant Title : VOC Analysis

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.
11.295	3.98 ug/L	41316	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	94
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, propyl-	10.906	2.9	ug/L	30172	3	11.812	519489	50.0
Benzene, 1-ethy...	11.295	4.0	ug/L	41316	3	11.812	519489	50.0