

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
 Data File : VU047929.D
 Acq On : 12 Apr 2022 00:32
 Operator : SY/MD
 Sample : N2293-17ME
 Misc : 6.65g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNP5ME

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\SFAMULM032422WMA.M
 Title : VOC Analysis

Signal : TIC: VU047929.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	73	80	108	rVB	95143	195442	10.67%	1.329%
2	2.539	361	373	386	rBV	267614	461861	25.21%	3.141%
3	3.105	544	549	550	rBV2	659	538	0.03%	0.004%
4	3.166	561	568	569	rBV2	419	462	0.03%	0.003%
5	3.324	612	617	621	rBV3	440	502	0.03%	0.003%
6	3.363	627	629	631	rVB2	268	108	0.01%	0.001%
7	3.411	636	644	645	rBV2	632	528	0.03%	0.004%
8	3.491	666	669	671	rBV2	218	130	0.01%	0.001%
9	3.507	671	674	676	rVV2	256	132	0.01%	0.001%
10	3.562	684	691	696	rBV2	359	554	0.03%	0.004%
11	3.662	717	722	723	rBV2	901	469	0.03%	0.003%
12	3.761	751	753	755	rBV	134	81	0.00%	0.001%
13	3.800	761	765	768	rVB2	311	198	0.01%	0.001%
14	3.822	768	772	774	rBV	161	129	0.01%	0.001%
15	3.864	782	785	787	rBV	294	174	0.01%	0.001%
16	3.887	790	792	795	rVV2	250	108	0.01%	0.001%
17	3.932	805	806	808	rBV	167	75	0.00%	0.001%
18	3.945	808	810	812	rVB	272	110	0.01%	0.001%
19	3.970	815	818	822	rVB2	187	159	0.01%	0.001%
20	4.031	834	837	839	rBV3	191	110	0.01%	0.001%
21	4.121	861	865	866	rBV2	259	181	0.01%	0.001%
22	4.176	879	882	884	rBV	245	166	0.01%	0.001%
23	4.250	902	905	906	rBV	246	114	0.01%	0.001%
24	4.379	941	945	946	rBV	301	180	0.01%	0.001%
25	4.443	960	965	968	rVB2	280	199	0.01%	0.001%
26	4.462	968	971	973	rBV	260	167	0.01%	0.001%
27	4.559	998	1001	1003	rBV2	352	199	0.01%	0.001%
28	4.633	1010	1024	1068	rBV	138466	447578	24.43%	3.044%
29	5.060	1140	1157	1182	rBV	270982	618990	33.78%	4.209%
30	5.199	1197	1200	1201	rBV	240	117	0.01%	0.001%
31	5.289	1224	1228	1231	rBV2	649	556	0.03%	0.004%
32	5.571	1315	1316	1317	rBV2	341	129	0.01%	0.001%
33	5.719	1340	1362	1374	rBV2	608708	1615946	88.19%	10.989%
34	5.909	1418	1421	1424	rBV2	374	267	0.01%	0.002%
35	5.973	1435	1441	1446	rBV4	1018	1316	0.07%	0.009%
36	6.057	1463	1467	1474	rBV2	276	323	0.02%	0.002%

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Instrument :
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 ClientSampleId :
 ETNP5ME

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\SFAMULM032422WMA.M
 Title : VOC Analysis

37	6.131	1478	1490	1496	rBV5	5738	10516	0.57%	0.072%
38	6.247	1512	1526	1548	rBV	577717	1153551	62.96%	7.845%
39	6.420	1578	1580	1587	rVB3	519	441	0.02%	0.003%
40	6.449	1587	1589	1591	rBV2	391	220	0.01%	0.001%
41	6.533	1605	1615	1629	rVB8	3163	6728	0.37%	0.046%
42	6.594	1629	1634	1635	rBV	783	571	0.03%	0.004%
43	6.690	1649	1664	1682	rBV	358466	725281	39.58%	4.932%
44	6.861	1714	1717	1722	rVB2	175	130	0.01%	0.001%
45	6.890	1722	1726	1729	rBV3	196	171	0.01%	0.001%
46	6.932	1736	1739	1740	rBV	145	88	0.00%	0.001%
47	7.063	1768	1780	1792	rVB7	2180	4452	0.24%	0.030%
48	7.186	1807	1818	1830	rBV3	8514	18546	1.01%	0.126%
49	7.375	1875	1877	1878	rBV	226	83	0.00%	0.001%
50	7.430	1888	1894	1898	rBV4	423	385	0.02%	0.003%
51	7.446	1898	1899	1900	rBV4	308	109	0.01%	0.001%
52	7.497	1906	1915	1924	rBV7	7764	16072	0.88%	0.109%
53	7.565	1926	1936	1955	rVB	169993	329581	17.99%	2.241%
54	7.694	1968	1976	1991	rBV4	2321	4841	0.26%	0.033%
55	7.809	2007	2012	2014	rBV2	511	398	0.02%	0.003%
56	7.899	2017	2040	2055	rBV	699618	1279376	69.82%	8.700%
57	8.182	2115	2128	2156	rBV	114857	237229	12.95%	1.613%
58	8.366	2178	2185	2198	rVB6	6837	13967	0.76%	0.095%
59	8.414	2198	2200	2202	rBV2	343	152	0.01%	0.001%
60	8.581	2242	2252	2259	rBV	3949	7747	0.42%	0.053%
61	8.652	2260	2274	2301	rVV	540029	1091515	59.57%	7.423%
62	9.076	2404	2406	2407	rBV	208	94	0.01%	0.001%
63	9.366	2490	2496	2499	rBV6	1297	1464	0.08%	0.010%
64	9.423	2500	2514	2518	rBV	910512	1577640	86.10%	10.729%
65	9.632	2576	2579	2583	rBV2	388	323	0.02%	0.002%
66	9.700	2591	2600	2612	rVB4	5592	9112	0.50%	0.062%
67	9.751	2612	2616	2620	rBV3	410	396	0.02%	0.003%
68	9.857	2647	2649	2651	rBV	182	104	0.01%	0.001%
69	9.935	2671	2673	2679	rVB3	350	264	0.01%	0.002%
70	9.999	2690	2693	2695	rVB2	210	116	0.01%	0.001%
71	10.012	2695	2697	2700	rVB2	176	98	0.01%	0.001%
72	10.105	2718	2726	2736	rBV5	3758	6230	0.34%	0.042%
73	10.179	2746	2749	2751	rBV2	283	152	0.01%	0.001%
74	10.192	2751	2753	2756	rBV	233	126	0.01%	0.001%
75	10.308	2785	2789	2792	rBV3	329	289	0.02%	0.002%
76	10.414	2819	2822	2823	rBV	182	96	0.01%	0.001%

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Instrument :
 MSVOA_U
 ClientSampleId :
 ETNP5ME

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\SFAMULM032422WMA.M
 Title : VOC Analysis

77	10.468	2837	2839	2840	rBV	474	236	0.01%	0.002%
78	10.529	2854	2858	2861	rBV3	346	276	0.02%	0.002%
79	10.658	2889	2898	2911	rBV8	5996	12440	0.68%	0.085%
80	10.764	2917	2931	2952	rBV	636843	1076389	58.75%	7.320%
81	10.983	2990	2999	3009	rBV6	5471	10800	0.59%	0.073%
82	11.256	3079	3084	3086	rBV	673	579	0.03%	0.004%
83	11.298	3091	3097	3104	rVB2	2346	2697	0.15%	0.018%
84	11.369	3116	3119	3122	rBV2	354	236	0.01%	0.002%
85	11.417	3130	3134	3139	rBV5	662	676	0.04%	0.005%
86	11.452	3140	3145	3147	rBV4	1640	1514	0.08%	0.010%
87	11.751	3231	3238	3245	rVB4	3341	4604	0.25%	0.031%
88	11.816	3245	3258	3273	rBV	1158942	1832300	100.00%	12.460%
89	12.195	3363	3376	3396	rBV	855421	1400279	76.42%	9.522%
90	12.398	3422	3439	3450	rVB2	17392	38635	2.11%	0.263%
91	12.468	3454	3461	3465	rBV3	2941	4169	0.23%	0.028%
92	12.539	3482	3483	3485	rBV	394	185	0.01%	0.001%
93	12.574	3487	3494	3503	rVB2	5286	7611	0.42%	0.052%
94	12.970	3607	3617	3628	rBV	129935	203605	11.11%	1.385%
95	13.330	3720	3729	3739	rBV	39034	62511	3.41%	0.425%
96	14.494	4082	4091	4103	rVB4	34745	56776	3.10%	0.386%
97	14.668	4139	4145	4157	rVB2	7674	11639	0.64%	0.079%
98	14.809	4183	4189	4198	rVB2	6824	9721	0.53%	0.066%
99	15.414	4370	4377	4388	rVB	17136	25779	1.41%	0.175%
100	15.545	4409	4418	4430	rBV2	60011	94375	5.15%	0.642%

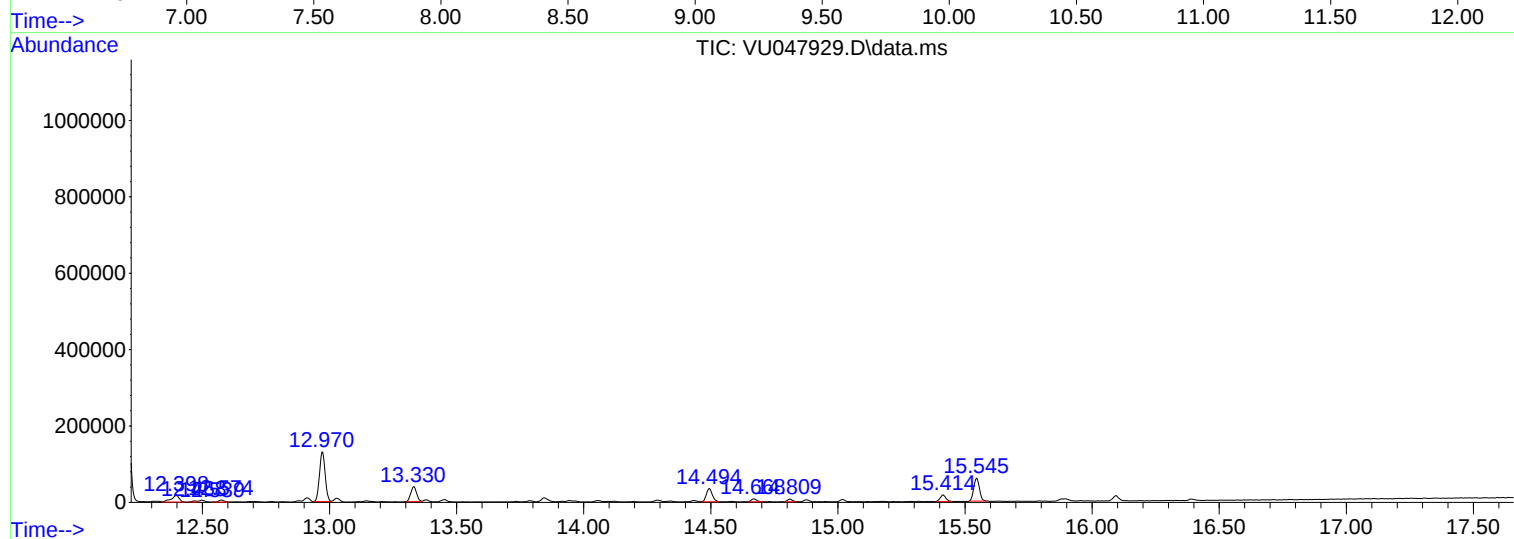
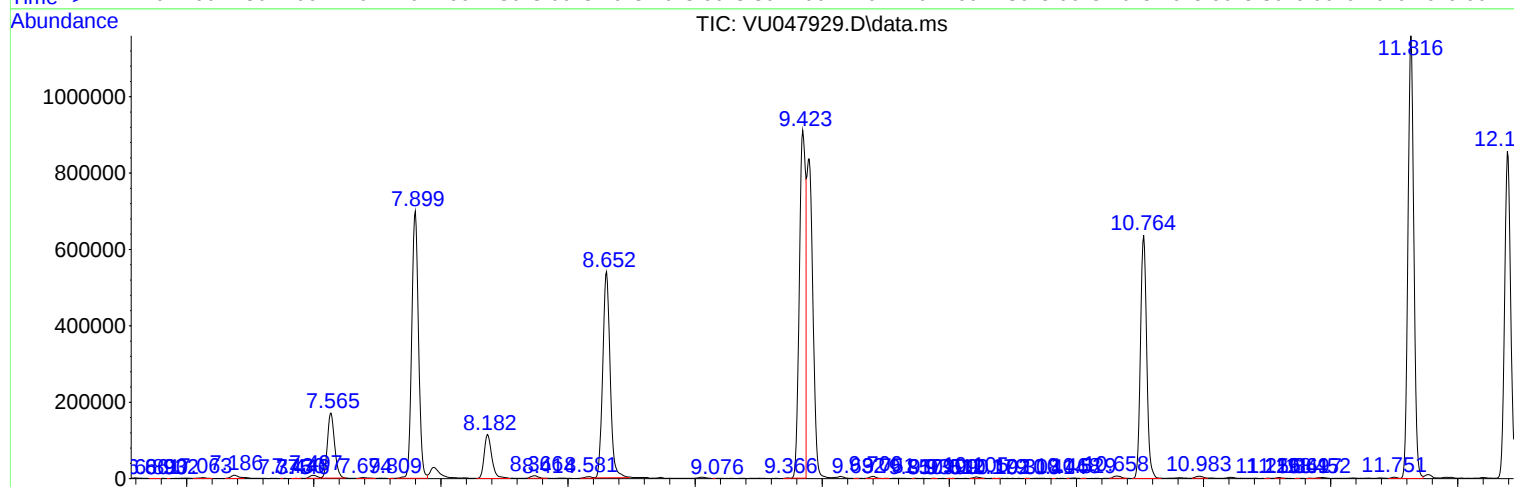
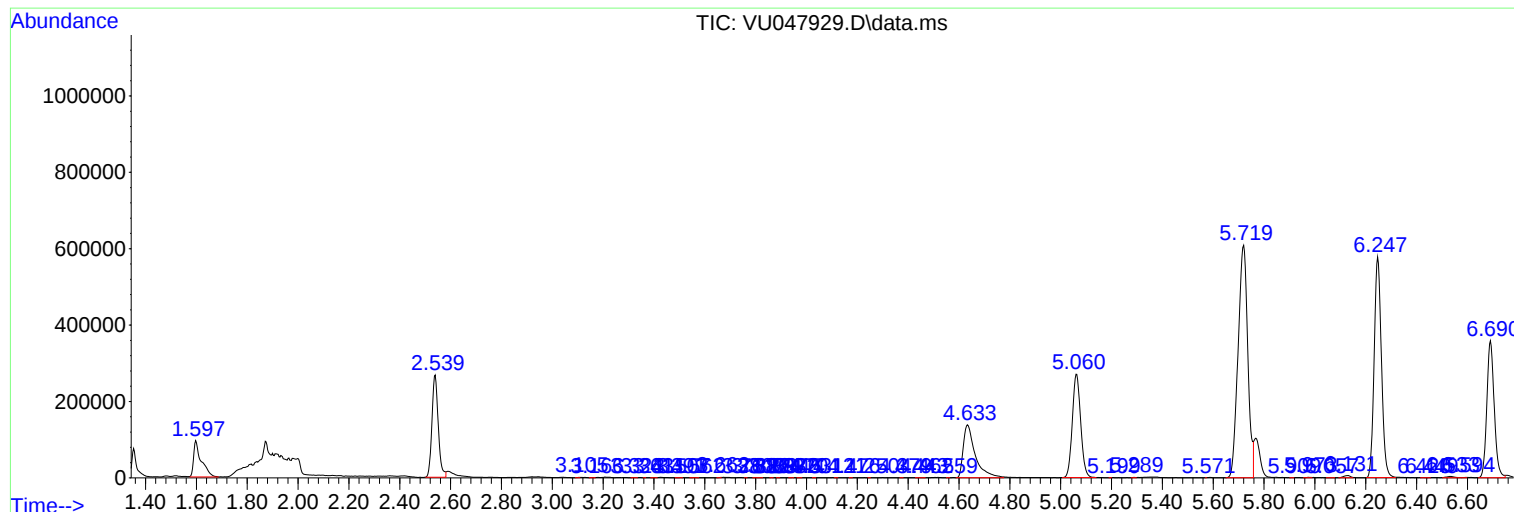
Sum of corrected areas: 14704984

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ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP5ME

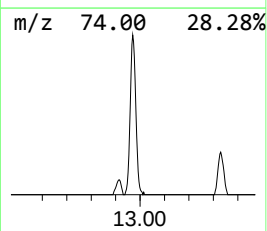
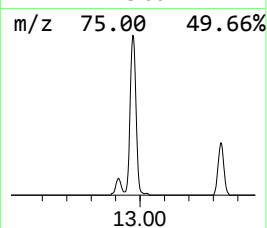
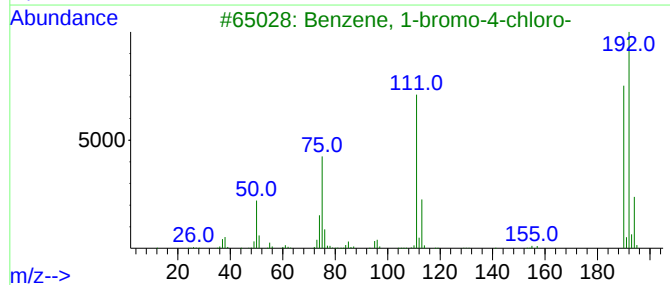
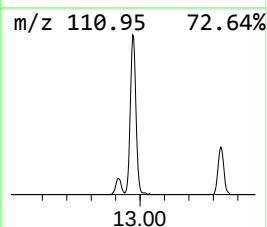
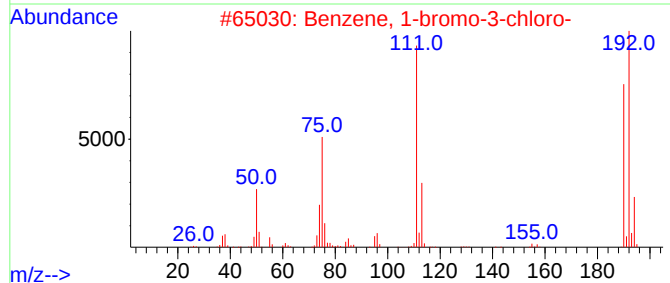
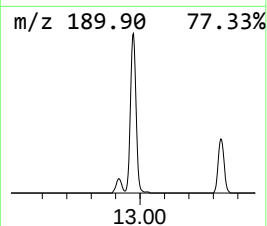
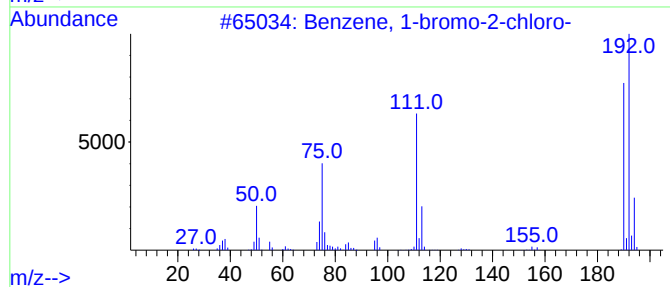
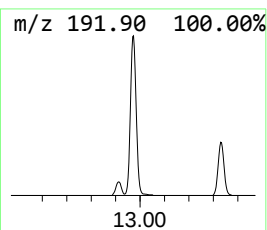
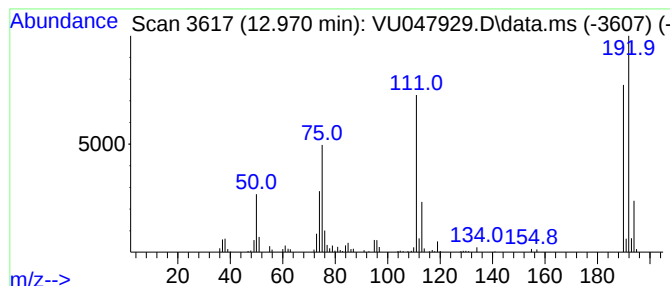
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Benzene, 1-bromo-2-chloro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.970	5.56 ug/L	203605	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-bromo-2-chloro-	190	C6H4BrCl	000694-80-4	98
2			Benzene, 1-bromo-3-chloro-	190	C6H4BrCl	000108-37-2	98
3			Benzene, 1-bromo-4-chloro-	190	C6H4BrCl	000106-39-8	98
4			Benzene, 1-bromo-2-chloro-	190	C6H4BrCl	000694-80-4	98
5			Benzene, 1-bromo-3-chloro-	190	C6H4BrCl	000108-37-2	98



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Instrument :
MSVOA_U
ClientSampleId :
ETNP5ME

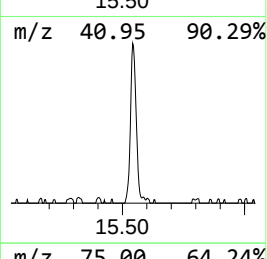
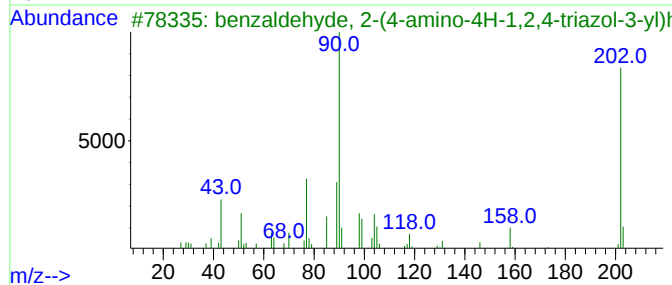
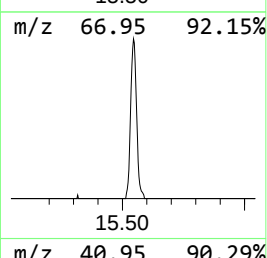
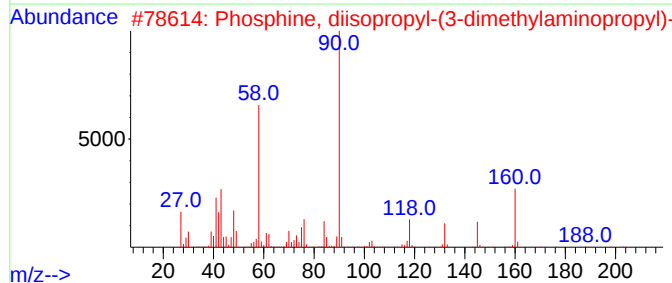
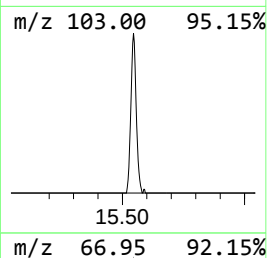
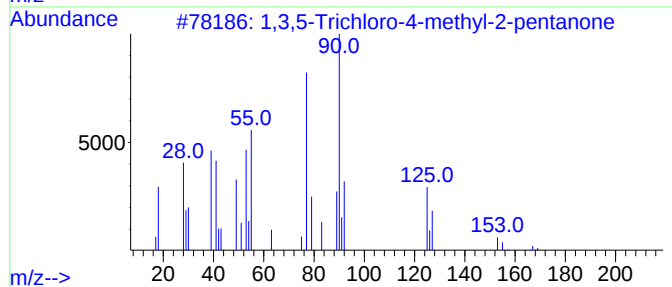
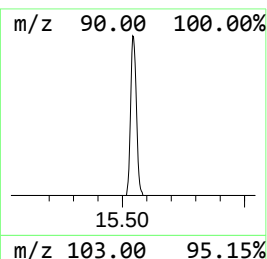
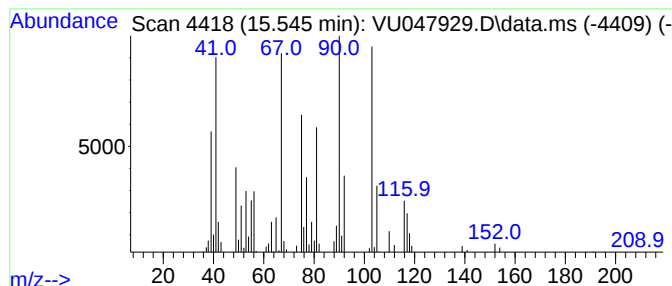
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.545	2.58 ug/L	94375	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3,5-Trichloro-4-methyl-2-penta...	202	C6H9Cl3O	1000140-03-8	30
2			Phosphine, diisopropyl-(3-dimeth...	203	C11H26NP	144533-36-8	25
3			benzaldehyde, 2-(4-amino-4H-1,2,...	202	C9H10N6	1000400-43-7	25
4			s-Triazole-3-carboxaldehyde, 5-p...	173	C9H7N3O	026899-64-9	25
5			4-(2-Aminoethyl)benzenesulfonamide	200	C8H12N2O2S	035303-76-5	25



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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
Benzene, 1-brom...	12.970	5.6	ug/L	203605	3	11.816	1832300	50.0
unknown-01	15.545	2.6	ug/L	94375	3	11.816	1832300	50.0