

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041522\
 Data File : VU048098.D
 Acq On : 15 Apr 2022 13:26
 Operator : SY/MD
 Sample : N2373-07ME
 Misc : 5.02g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFFD8ME

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: VU048098.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	111	rVB	36414	81307	10.27%	1.216%
2	2.475	351	353	356	rBV3	444	273	0.03%	0.004%
3	2.543	363	374	386	rBV	93389	162494	20.52%	2.431%
4	2.884	476	480	481	rBV	303	221	0.03%	0.003%
5	2.929	485	494	496	rBV3	543	846	0.11%	0.013%
6	3.038	520	528	550	rVB9	3150	8540	1.08%	0.128%
7	3.183	558	573	591	rBV2	21766	59560	7.52%	0.891%
8	3.478	662	665	669	rVB3	413	257	0.03%	0.004%
9	3.514	673	676	682	rVB2	346	344	0.04%	0.005%
10	3.819	766	771	774	rBV2	293	309	0.04%	0.005%
11	3.851	775	781	786	rVV4	752	756	0.10%	0.011%
12	3.925	800	804	807	rVB3	339	301	0.04%	0.005%
13	4.009	828	830	837	rVB2	288	217	0.03%	0.003%
14	4.054	842	844	850	rVB3	337	311	0.04%	0.005%
15	4.092	851	856	859	rBV	419	395	0.05%	0.006%
16	4.318	920	926	931	rBV2	261	421	0.05%	0.006%
17	4.440	958	964	968	rBV2	344	401	0.05%	0.006%
18	4.646	1014	1028	1082	rBV2	74529	318997	40.29%	4.773%
19	5.064	1141	1158	1185	rBV2	139644	326640	41.25%	4.887%
20	5.298	1226	1231	1238	rVB4	525	694	0.09%	0.010%
21	5.337	1238	1243	1244	rBV3	439	436	0.06%	0.007%
22	5.546	1304	1308	1315	rVB2	213	318	0.04%	0.005%
23	5.600	1320	1325	1329	rBV2	273	274	0.03%	0.004%
24	5.719	1343	1362	1394	rBV2	295775	791800	100.00%	11.847%
25	5.829	1394	1396	1402	rVB2	349	236	0.03%	0.004%
26	5.980	1430	1443	1463	rBV3	13536	33921	4.28%	0.508%
27	6.247	1512	1526	1551	rBV	290777	591032	74.64%	8.843%
28	6.459	1588	1592	1594	rBV2	390	229	0.03%	0.003%
29	6.526	1603	1613	1623	rBV6	4906	9651	1.22%	0.144%
30	6.604	1627	1637	1650	rVV2	6120	13428	1.70%	0.201%
31	6.690	1650	1664	1685	rVB	186535	382885	48.36%	5.729%
32	6.787	1690	1694	1695	rBV3	450	307	0.04%	0.005%
33	6.848	1710	1713	1717	rVB	428	322	0.04%	0.005%
34	6.967	1746	1750	1751	rBV	335	232	0.03%	0.003%
35	7.051	1771	1776	1780	rVV3	517	382	0.05%	0.006%
36	7.083	1783	1786	1793	rVB3	379	307	0.04%	0.005%

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 ALS Vial : 6 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
 BFFD8ME

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	7.218	1810	1828	1847	rBV7	9170	32129	4.06%	0.481%
38	7.491	1910	1913	1914	rBV	567	297	0.04%	0.004%
39	7.568	1924	1937	1958	rBV2	76033	149801	18.92%	2.241%
40	7.684	1967	1973	1974	rBV	1241	791	0.10%	0.012%
41	7.797	1996	2008	2016	rBV3	6718	13673	1.73%	0.205%
42	7.899	2027	2040	2056	rBV	255637	465286	58.76%	6.961%
43	8.182	2116	2128	2149	rBV2	49978	105157	13.28%	1.573%
44	8.330	2171	2174	2175	rBV2	376	214	0.03%	0.003%
45	8.350	2175	2180	2185	rBV4	1097	1242	0.16%	0.019%
46	8.440	2202	2208	2209	rBV	420	396	0.05%	0.006%
47	8.546	2237	2241	2242	rBV	313	235	0.03%	0.004%
48	8.581	2248	2252	2255	rVB	409	366	0.05%	0.005%
49	8.665	2260	2278	2309	rBV	270085	616155	77.82%	9.219%
50	8.932	2352	2361	2365	rBV5	1275	2262	0.29%	0.034%
51	9.070	2399	2404	2408	rBV2	327	340	0.04%	0.005%
52	9.189	2435	2441	2443	rBV2	229	238	0.03%	0.004%
53	9.330	2483	2485	2492	rVB2	455	315	0.04%	0.005%
54	9.423	2498	2514	2548	rBV	358586	749001	94.59%	11.206%
55	9.575	2556	2561	2569	rVB3	507	750	0.09%	0.011%
56	9.697	2595	2599	2609	rVB6	760	854	0.11%	0.013%
57	9.858	2645	2649	2657	rVB2	369	499	0.06%	0.007%
58	9.896	2657	2661	2667	rBV	320	397	0.05%	0.006%
59	10.105	2721	2726	2728	rBV3	365	317	0.04%	0.005%
60	10.211	2755	2759	2765	rVB3	282	230	0.03%	0.003%
61	10.362	2802	2806	2809	rBV2	476	393	0.05%	0.006%
62	10.430	2822	2827	2830	rBV	313	314	0.04%	0.005%
63	10.620	2883	2886	2889	rBV2	410	305	0.04%	0.005%
64	10.661	2893	2899	2913	rVB7	2314	4196	0.53%	0.063%
65	10.767	2918	2932	2948	rBV	340137	549846	69.44%	8.227%
66	10.829	2948	2951	2955	rVB5	568	303	0.04%	0.005%
67	10.896	2964	2972	2975	rBV3	1393	1577	0.20%	0.024%
68	11.002	3002	3005	3009	rVB3	322	230	0.03%	0.003%
69	11.028	3009	3013	3017	rBV3	287	239	0.03%	0.004%
70	11.047	3017	3019	3023	rVB2	428	326	0.04%	0.005%
71	11.073	3023	3027	3028	rBV2	280	210	0.03%	0.003%
72	11.115	3034	3040	3048	rBV6	2475	3279	0.41%	0.049%
73	11.208	3064	3069	3072	rBV3	438	290	0.04%	0.004%
74	11.308	3094	3100	3112	rVB3	844	1394	0.18%	0.021%
75	11.356	3112	3115	3117	rBV2	360	284	0.04%	0.004%
76	11.372	3117	3120	3123	rBV3	650	485	0.06%	0.007%

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 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFFD8ME

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	11.414	3130	3133	3135	rBV2	460	248	0.03%	0.004%
78	11.459	3138	3147	3152	rBV5	1511	2069	0.26%	0.031%
79	11.578	3180	3184	3190	rVB2	635	686	0.09%	0.010%
80	11.697	3214	3221	3227	rBV6	1153	1658	0.21%	0.025%
81	11.751	3232	3238	3246	rVV4	1820	2575	0.33%	0.039%
82	11.816	3246	3258	3277	rVV	411405	674397	85.17%	10.090%
83	11.886	3278	3280	3287	rVB5	770	633	0.08%	0.009%
84	11.973	3302	3307	3312	rVB3	1253	1435	0.18%	0.021%
85	12.198	3363	3377	3395	rVB	290074	477616	60.32%	7.146%
86	12.314	3410	3413	3415	rBV	416	219	0.03%	0.003%
87	12.533	3477	3481	3486	rBV3	266	302	0.04%	0.005%
88	12.677	3521	3526	3530	rBV3	303	339	0.04%	0.005%
89	12.774	3548	3556	3564	rVB3	1911	2778	0.35%	0.042%
90	12.890	3588	3592	3598	rVB2	298	324	0.04%	0.005%
91	12.918	3598	3601	3603	rBV2	280	226	0.03%	0.003%
92	13.031	3633	3636	3640	rVB2	331	247	0.03%	0.004%
93	13.060	3640	3645	3656	rBV3	402	900	0.11%	0.013%
94	13.224	3693	3696	3703	rVB3	637	762	0.10%	0.011%
95	13.848	3880	3890	3905	rBV	8775	14016	1.77%	0.210%
96	14.333	4035	4041	4051	rVB4	2834	3902	0.49%	0.058%
97	14.401	4059	4062	4065	rBV3	396	309	0.04%	0.005%
98	14.443	4072	4075	4077	rVB	411	212	0.03%	0.003%
99	14.574	4111	4116	4128	rVB2	2455	3994	0.50%	0.060%
100	14.700	4153	4155	4159	rBV2	498	281	0.04%	0.004%

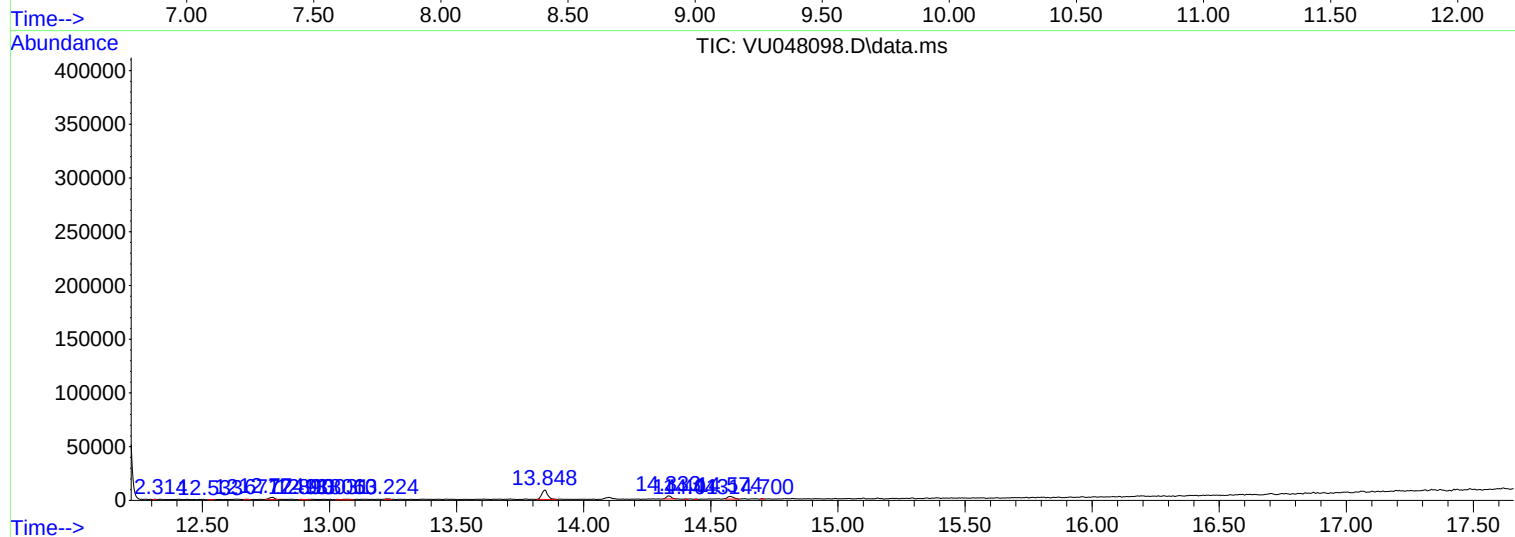
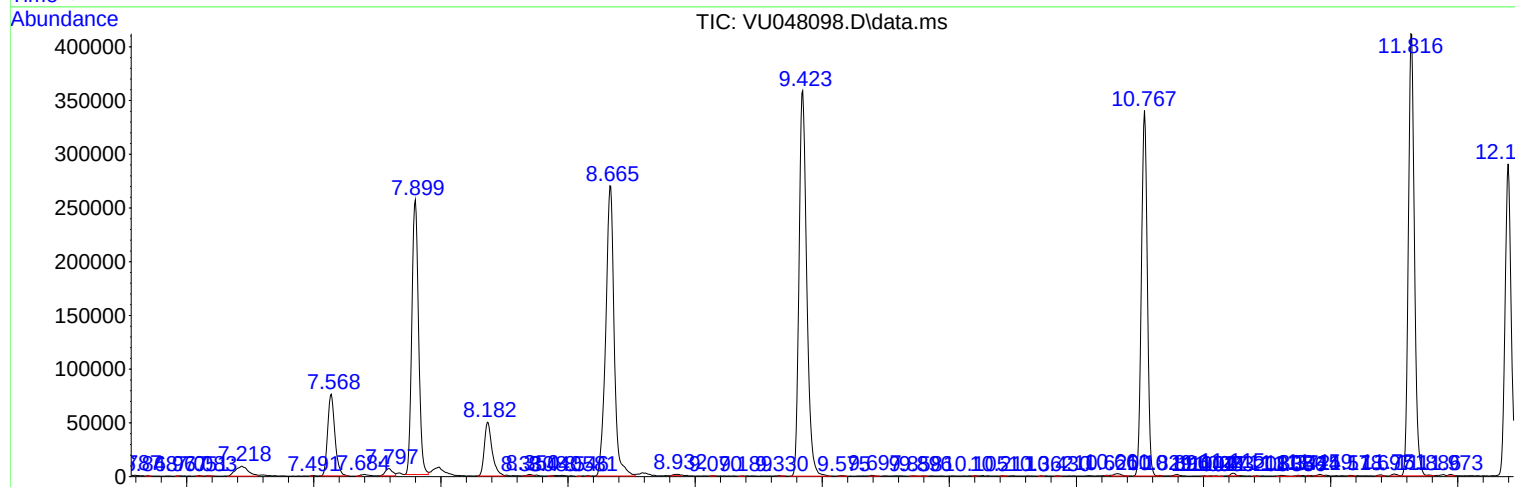
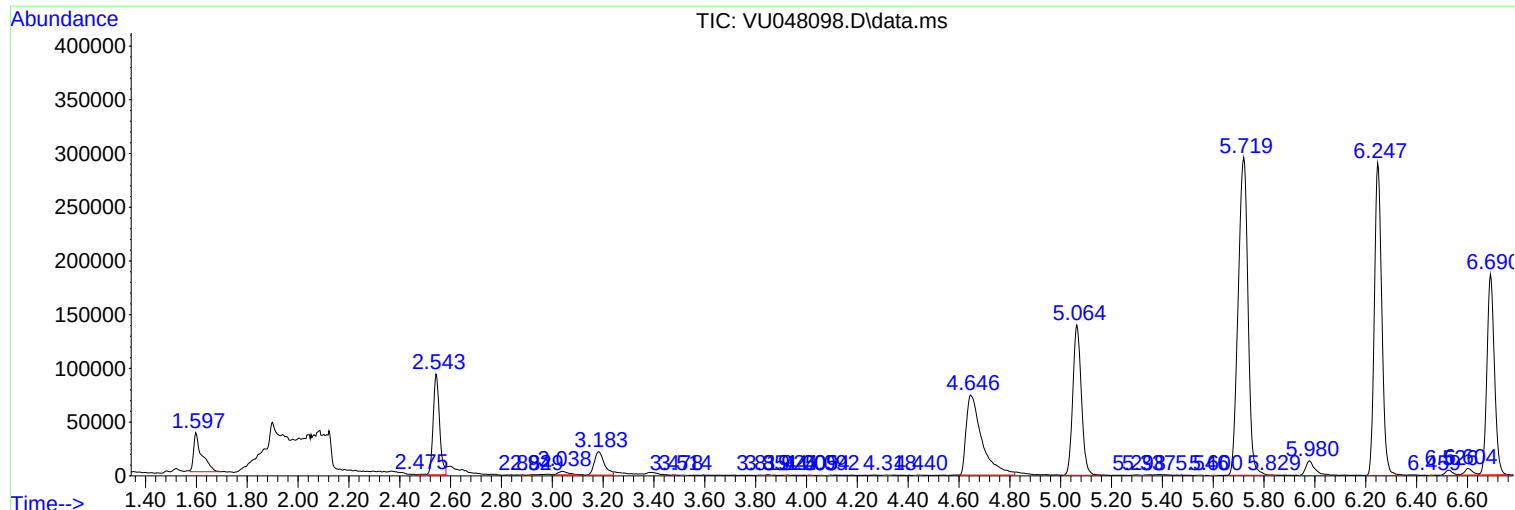
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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFFD8ME

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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Sample : N2373-07ME
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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFFD8ME

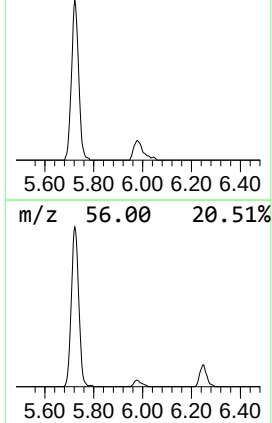
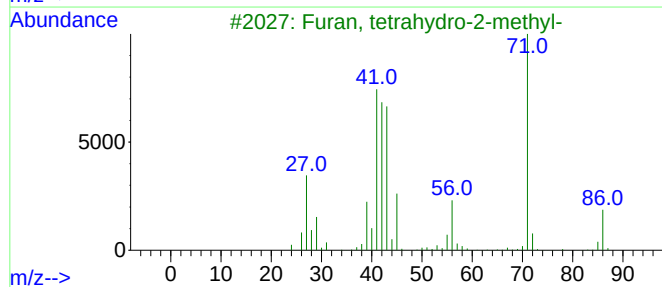
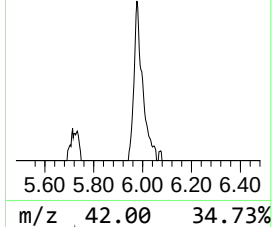
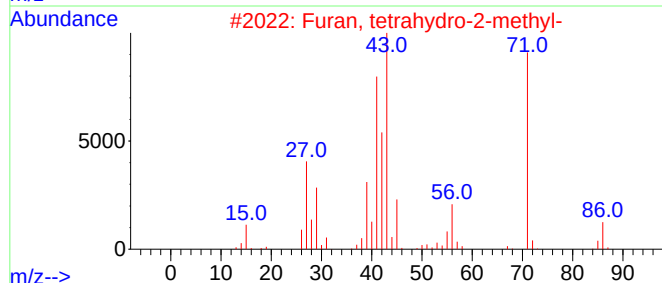
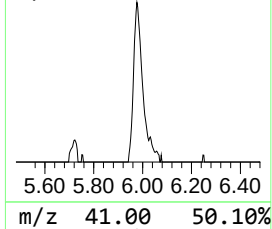
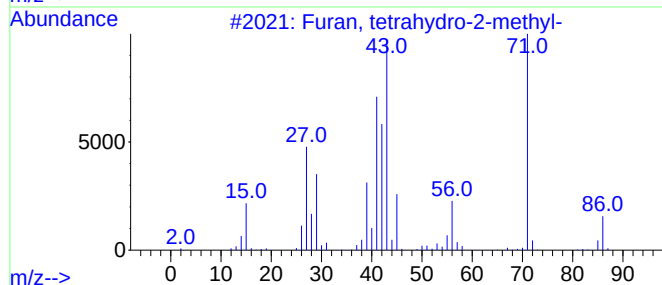
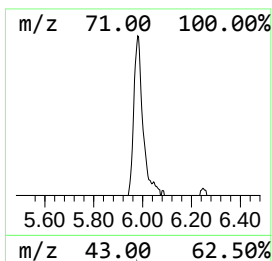
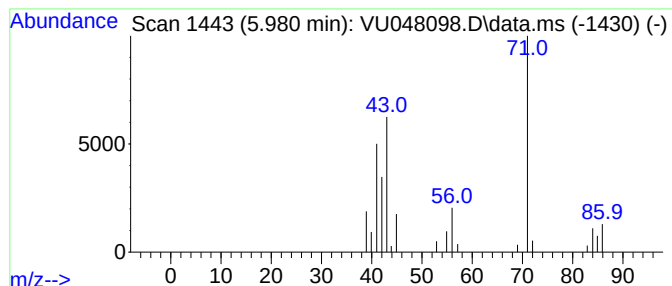
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Furan, tetrahydro-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.980	2.87 ug/L	33921	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	90
2			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	87
3			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	80
4			Pentane, 2-methyl-	86	C6H14	000107-83-5	53
5			trans-3-Penten-2-ol	86	C5H10O	003899-34-1	50



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Misc : 5.02g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFFD8ME

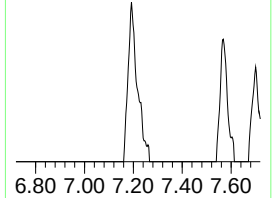
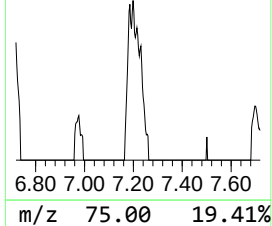
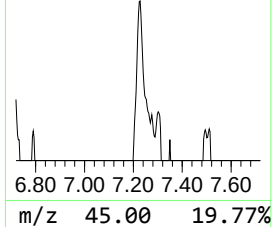
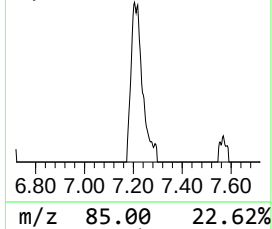
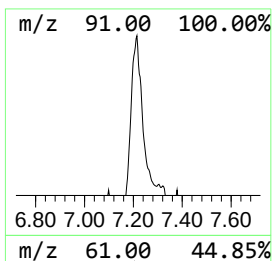
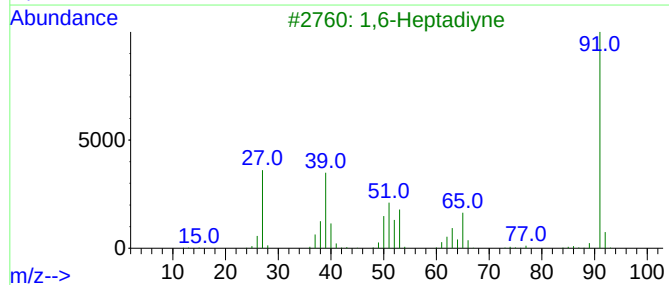
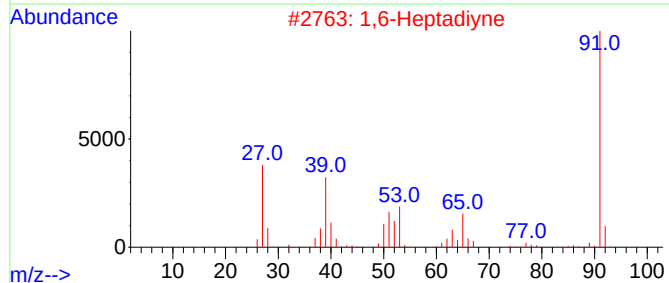
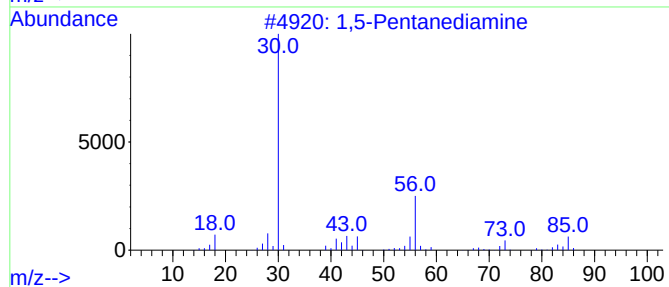
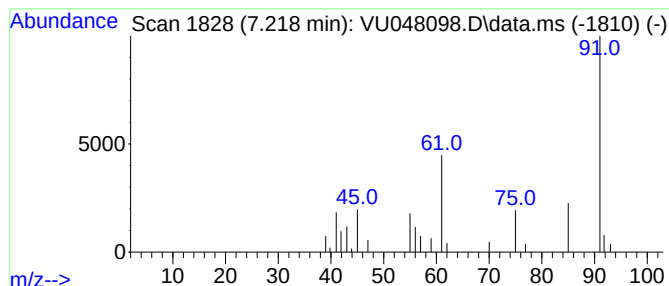
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.218	2.72 ug/L	32129	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,5-Pentanediamine	102	C5H14N2	000462-94-2	9
2			1,6-Heptadiyne	92	C7H8	002396-63-6	5
3			1,6-Heptadiyne	92	C7H8	002396-63-6	5
4			1,6-Heptadiyne	92	C7H8	002396-63-6	4
5			1-Propanol, 3-amino-	75	C3H9NO	000156-87-6	4



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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
Furan, tetrahyd...	5.980	2.9	ug/L	33921	1	6.247	591032	50.0
unknown-01	7.218	2.7	ug/L	32129	1	6.247	591032	50.0