

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV031022\
 Data File : VV024922.D
 Acq On : 10 Mar 2022 17:43
 Operator : SY/MD
 Sample : N1816-20ME
 Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DBSE5ME

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_V\Method\SFAMVLM022822WMA.M
 Title : VOC Analysis

Signal : TIC: VV024922.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.307	75	83	102	rVB	333093	412233	15.19%	2.885%
2	1.568	156	164	186	rVB	202856	289384	10.66%	2.025%
3	2.085	314	325	338	rBV	645354	918581	33.84%	6.428%
4	2.317	393	397	400	rBV3	535	432	0.02%	0.003%
5	2.372	412	414	418	rVB3	458	276	0.01%	0.002%
6	2.439	429	435	437	rBV3	556	532	0.02%	0.004%
7	2.963	594	598	601	rBV2	279	283	0.01%	0.002%
8	3.031	615	619	622	rVV2	301	248	0.01%	0.002%
9	3.632	803	806	811	rBV2	262	234	0.01%	0.002%
10	3.687	816	823	826	rVB2	231	236	0.01%	0.002%
11	3.764	843	847	851	rBV2	270	294	0.01%	0.002%
12	3.902	878	890	947	rBV	112218	494555	18.22%	3.461%
13	4.343	1010	1027	1064	rVB	412384	1056273	38.91%	7.391%
14	4.651	1120	1123	1131	rVV4	357	443	0.02%	0.003%
15	4.703	1135	1139	1144	rBV3	249	258	0.01%	0.002%
16	4.899	1196	1200	1204	rVB2	258	238	0.01%	0.002%
17	5.037	1224	1243	1272	rBV2	1094048	2714479	100.00%	18.995%
18	5.342	1327	1338	1347	rBV6	4613	11673	0.43%	0.082%
19	5.494	1382	1385	1389	rVB3	382	310	0.01%	0.002%
20	5.513	1389	1391	1397	rVB	384	263	0.01%	0.002%
21	5.542	1397	1400	1403	rBV	498	454	0.02%	0.003%
22	5.616	1412	1423	1446	rBV	65498	142541	5.25%	0.997%
23	5.902	1501	1512	1532	rBV	46400	101338	3.73%	0.709%
24	6.066	1549	1563	1602	rVB	567279	1201665	44.27%	8.409%
25	6.246	1617	1619	1623	rVB3	452	307	0.01%	0.002%
26	6.294	1631	1634	1638	rBV3	332	237	0.01%	0.002%
27	6.339	1642	1648	1652	rBV	371	366	0.01%	0.003%
28	6.375	1656	1659	1667	rVB2	343	244	0.01%	0.002%
29	6.420	1667	1673	1677	rBV2	244	374	0.01%	0.003%
30	6.542	1702	1711	1716	rBV3	265	461	0.02%	0.003%
31	6.641	1735	1742	1747	rBV7	2399	3970	0.15%	0.028%
32	6.741	1771	1773	1776	rVB2	458	299	0.01%	0.002%
33	6.850	1799	1807	1812	rBV	237	314	0.01%	0.002%
34	6.982	1836	1848	1882	rBV	302446	609937	22.47%	4.268%
35	7.140	1896	1897	1904	rVB3	364	238	0.01%	0.002%
36	7.198	1908	1915	1917	rVV	988	1053	0.04%	0.007%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022822WMA.M
 Title : VOC Analysis

37	7.211	1917	1919	1927	rVB3	1113	823	0.03%	0.006%
38	7.313	1936	1951	1970	rBV	1270439	2272584	83.72%	15.902%
39	7.619	2033	2046	2087	rBV2	177028	396848	14.62%	2.777%
40	7.937	2137	2145	2147	rBV2	604	664	0.02%	0.005%
41	7.979	2152	2158	2166	rVB3	2108	2720	0.10%	0.019%
42	8.095	2183	2194	2196	rBV	178711	240192	8.85%	1.681%
43	8.407	2289	2291	2297	rBV2	405	354	0.01%	0.002%
44	8.609	2348	2354	2355	rBV	412	291	0.01%	0.002%
45	8.857	2420	2431	2458	rBV	94263	190106	7.00%	1.330%
46	9.120	2509	2513	2515	rBV2	539	429	0.02%	0.003%
47	9.149	2515	2522	2526	rBV5	848	963	0.04%	0.007%
48	9.262	2553	2557	2561	rVV2	235	275	0.01%	0.002%
49	9.455	2612	2617	2620	rBV2	349	251	0.01%	0.002%
50	9.561	2645	2650	2654	rVB3	260	229	0.01%	0.002%
51	9.683	2681	2688	2693	rBV3	501	552	0.02%	0.004%
52	9.805	2720	2726	2728	rBV2	227	242	0.01%	0.002%
53	9.841	2734	2737	2746	rVV	156	233	0.01%	0.002%
54	10.127	2816	2826	2835	rBV3	8826	13712	0.51%	0.096%
55	10.223	2839	2856	2874	rBV	620102	1125275	41.45%	7.874%
56	10.455	2925	2928	2929	rBV	528	301	0.01%	0.002%
57	10.577	2956	2966	2985	rVV6	4249	9706	0.36%	0.068%
58	10.664	2985	2993	2997	rVV4	920	1257	0.05%	0.009%
59	10.776	3024	3028	3029	rBV2	369	285	0.01%	0.002%
60	10.876	3053	3059	3062	rBV4	580	697	0.03%	0.005%
61	10.915	3063	3071	3081	rVV3	7170	11378	0.42%	0.080%
62	11.037	3098	3109	3117	rBV3	1475	2326	0.09%	0.016%
63	11.143	3134	3142	3154	rVB4	3775	6272	0.23%	0.044%
64	11.252	3166	3176	3193	rBV	113250	181149	6.67%	1.268%
65	11.323	3193	3198	3206	rVB5	1638	2383	0.09%	0.017%
66	11.384	3206	3217	3224	rBV4	3677	6550	0.24%	0.046%
67	11.426	3224	3230	3241	rVB3	5554	8298	0.31%	0.058%
68	11.567	3271	3274	3280	rBV5	467	534	0.02%	0.004%
69	11.625	3280	3292	3313	rBV	1157624	1826775	67.30%	12.783%
70	11.786	3335	3342	3350	rVB6	2524	3936	0.15%	0.028%
71	11.847	3352	3361	3371	rVV7	1340	2743	0.10%	0.019%
72	11.998	3405	3408	3413	rVB3	360	298	0.01%	0.002%
73	12.046	3416	3423	3426	rBV4	469	634	0.02%	0.004%
74	12.085	3430	3435	3436	rBV	906	656	0.02%	0.005%
75	12.249	3479	3486	3493	rVV4	854	1189	0.04%	0.008%
76	12.294	3495	3500	3504	rVB2	478	461	0.02%	0.003%

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77	12.349	3511	3517	3519	rVV3	249	261	0.01%	0.002%
78	12.390	3526	3530	3534	rBV2	287	300	0.01%	0.002%
79	12.487	3552	3560	3562	rBV3	543	578	0.02%	0.004%
80	12.529	3570	3573	3579	rVB3	443	450	0.02%	0.003%
81	12.596	3585	3594	3603	rVV5	1379	2316	0.09%	0.016%
82	12.644	3603	3609	3613	rVB2	295	332	0.01%	0.002%
83	12.789	3651	3654	3658	rVB	392	274	0.01%	0.002%
84	13.040	3725	3732	3735	rBV2	249	300	0.01%	0.002%
85	13.072	3735	3742	3746	rBV	361	393	0.01%	0.003%
86	13.172	3769	3773	3776	rBV2	212	235	0.01%	0.002%
87	13.448	3854	3859	3868	rBV	442	619	0.02%	0.004%
88	13.548	3887	3890	3893	rVB2	362	232	0.01%	0.002%
89	13.911	3999	4003	4008	rBV3	383	422	0.02%	0.003%
90	14.024	4036	4038	4040	rBV	339	232	0.01%	0.002%
91	14.040	4041	4043	4047	rVB2	465	264	0.01%	0.002%
92	14.271	4111	4115	4121	rBV	365	448	0.02%	0.003%
93	14.400	4149	4155	4158	rBV2	372	459	0.02%	0.003%
94	14.422	4159	4162	4169	rVV3	301	429	0.02%	0.003%
95	14.741	4257	4261	4263	rBV2	349	277	0.01%	0.002%
96	15.230	4411	4413	4420	rVB2	484	452	0.02%	0.003%
97	15.631	4534	4538	4540	rBV2	495	411	0.02%	0.003%
98	15.683	4550	4554	4560	rBV3	694	792	0.03%	0.006%
99	16.117	4687	4689	4693	rBV2	482	299	0.01%	0.002%
100	16.271	4735	4737	4739	rBV	593	386	0.01%	0.003%

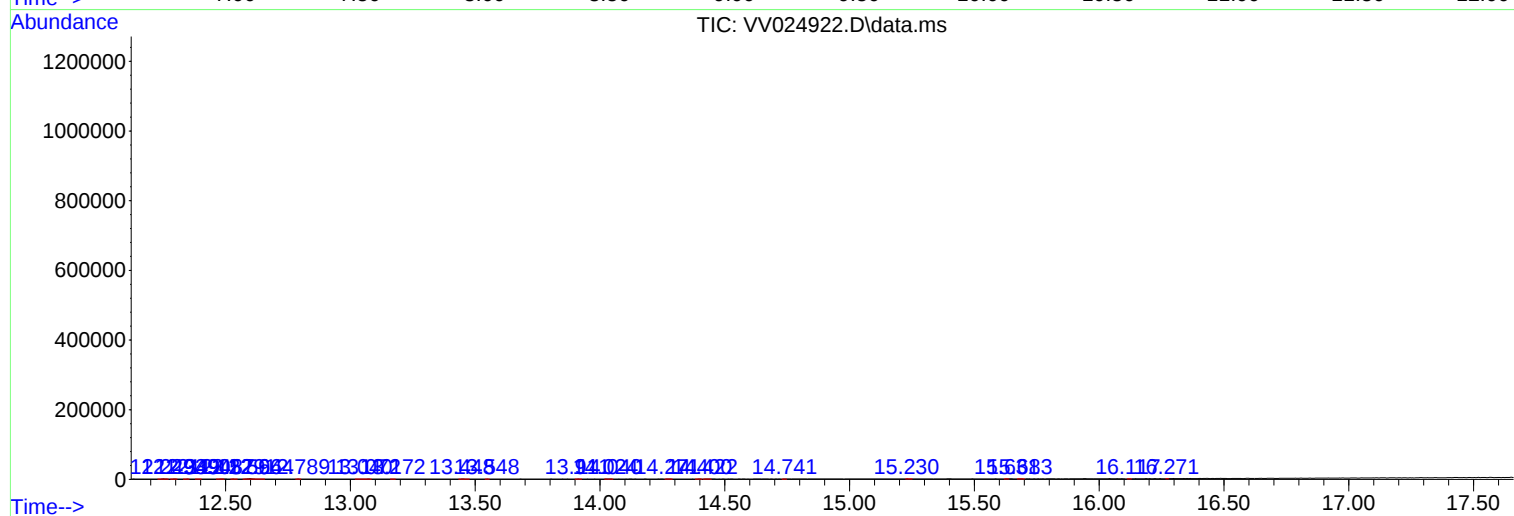
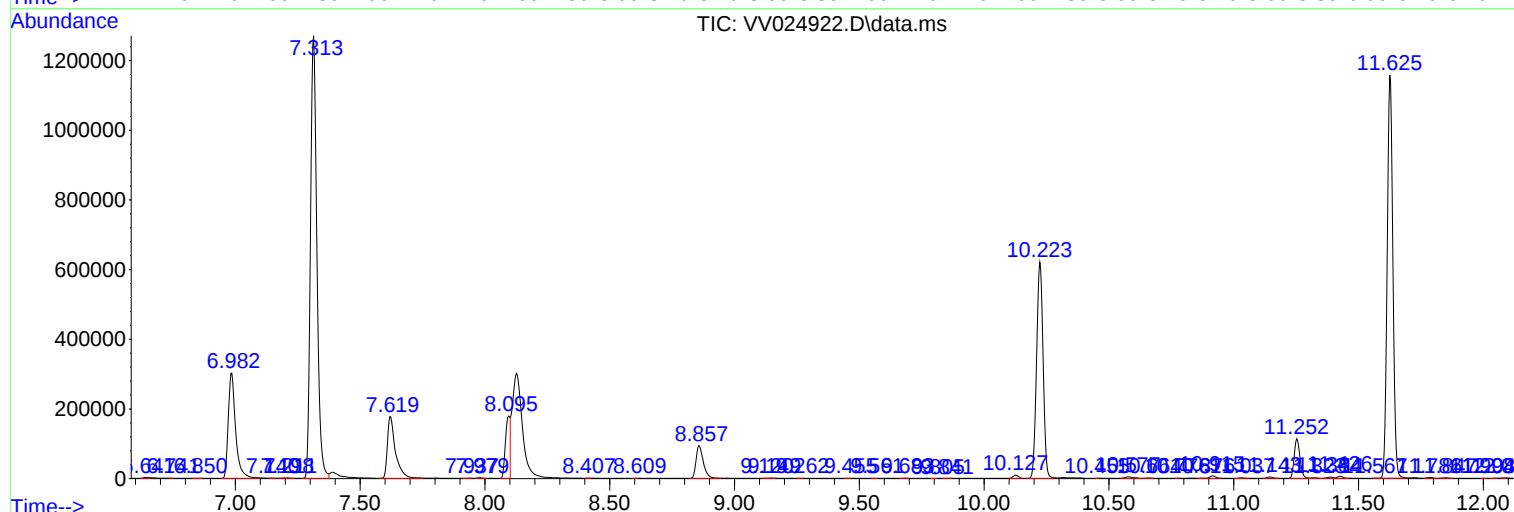
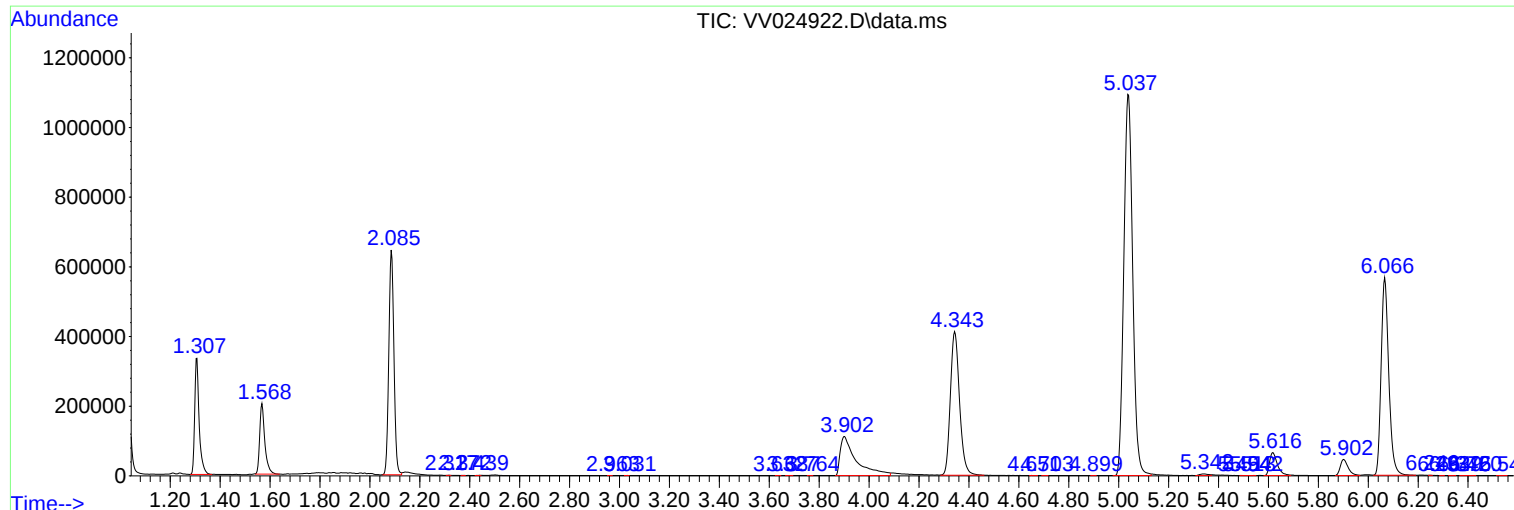
Sum of corrected areas: 14290755

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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBSE5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022822WMA.M
Quant Title : VOC Analysis

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



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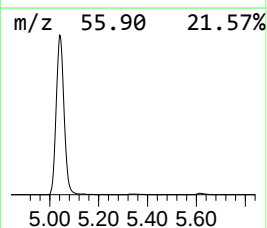
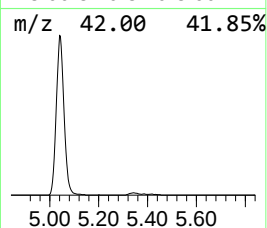
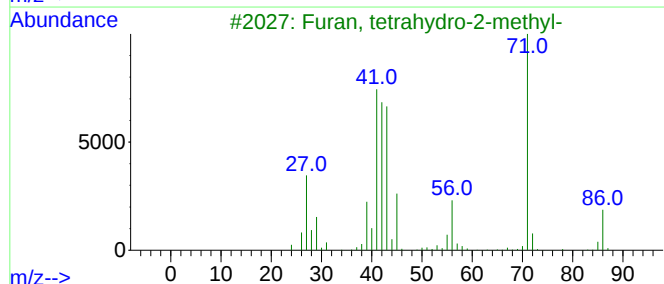
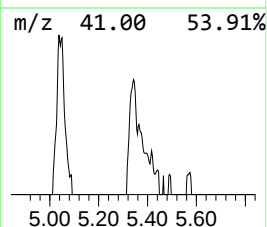
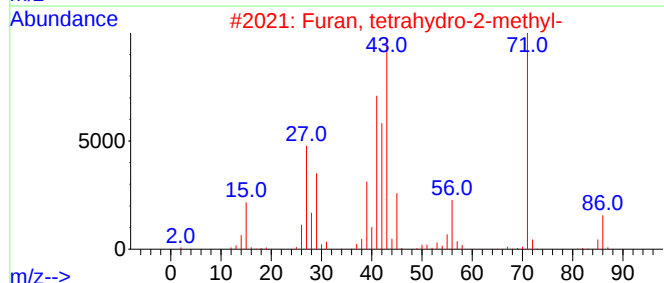
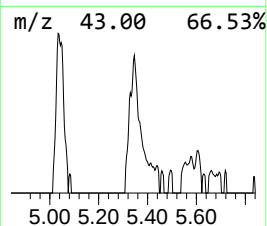
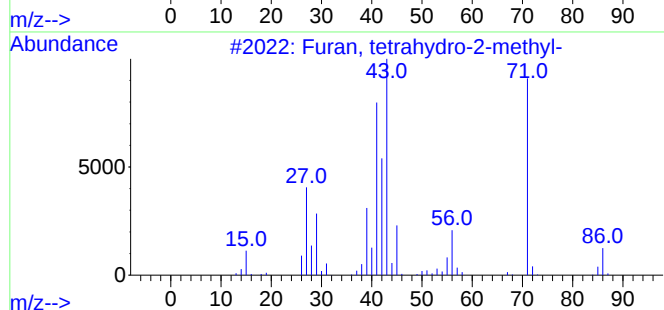
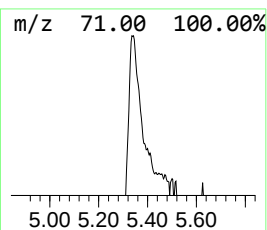
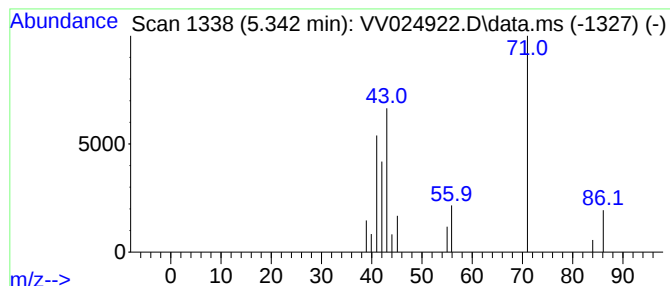
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022822WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Furan, tetrahydro-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.342	4.09 ug/L	11673	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	78
2			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	64
3			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	64
4			Pentane, 2-methyl-	86	C6H14	000107-83-5	9
5			Pentane, 2-methyl-	86	C6H14	000107-83-5	9



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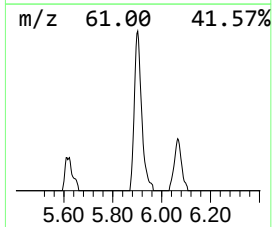
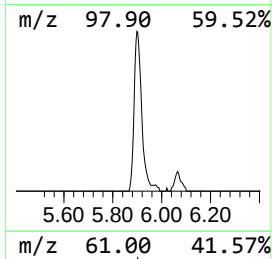
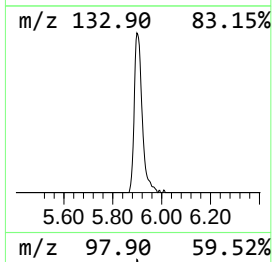
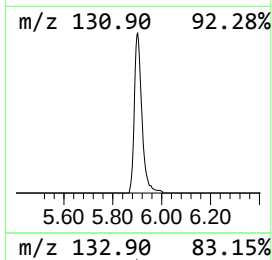
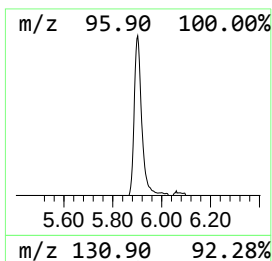
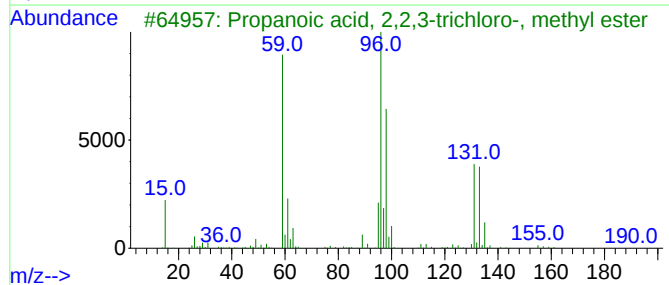
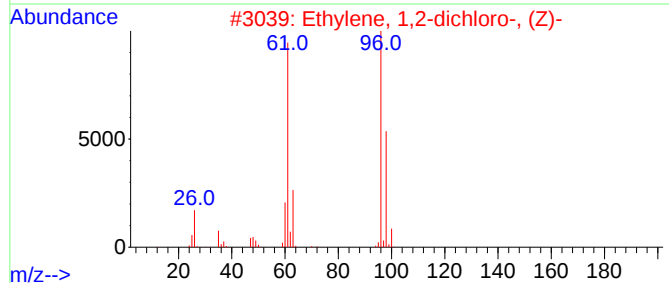
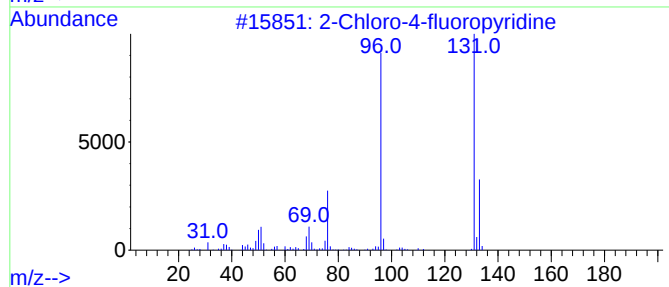
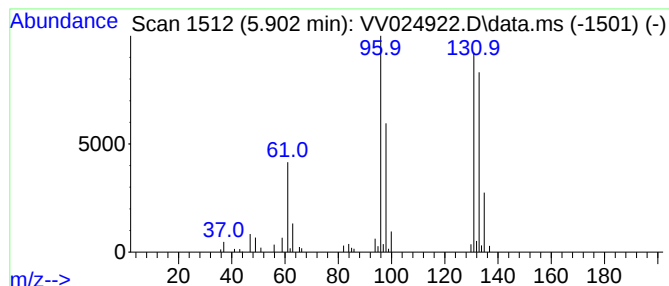
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022822WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.902	35.55 ug/L	101338	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	38
2			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
3			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	37
4			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	27
5			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	27



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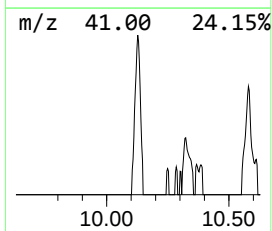
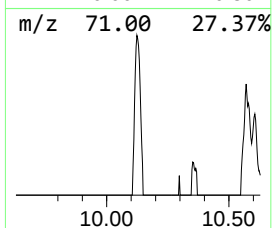
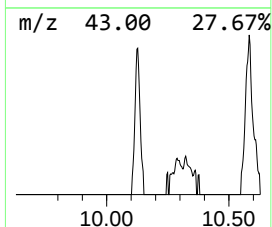
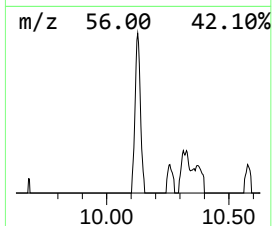
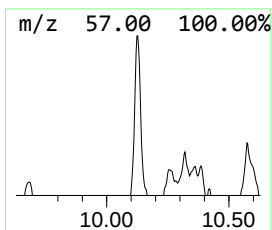
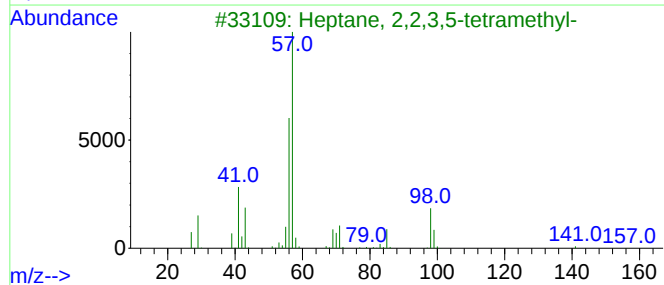
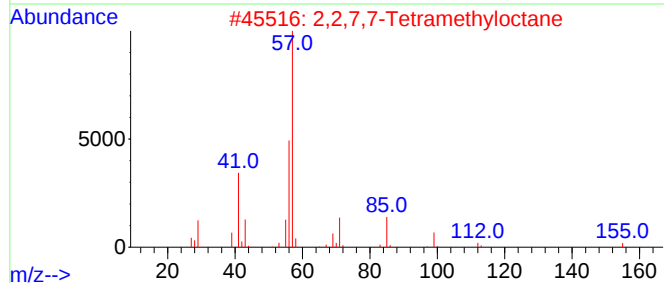
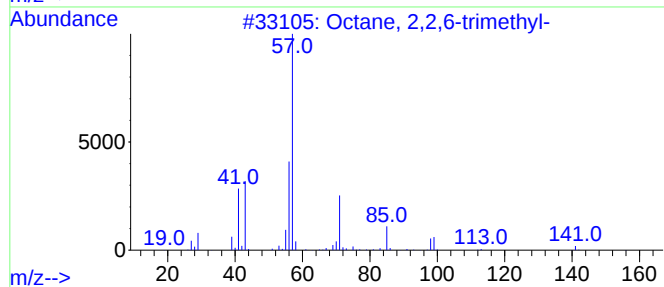
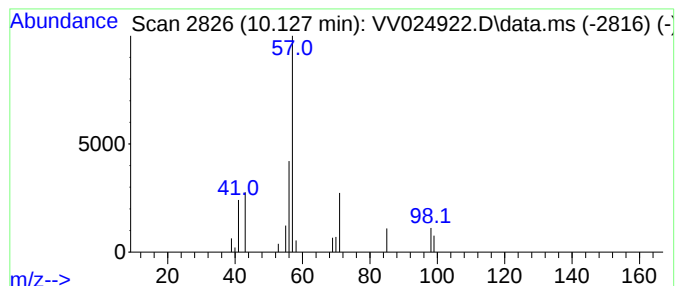
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Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.127	3.78 ug/L	13712	1,4-Dichlorobenzene-d4	11.252

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	78
2			2,2,7,7-Tetramethyloctane	170	C12H26	001071-31-4	64
3			Heptane, 2,2,3,5-tetramethyl-	156	C11H24	061868-42-6	59
4			Decane, 2,5,6-trimethyl-	184	C13H28	062108-23-0	53
5			Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV031022\
Data File : VV024922.D
Acq On : 10 Mar 2022 17:43
Operator : SY/MD
Sample : N1816-20ME
Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBSE5ME

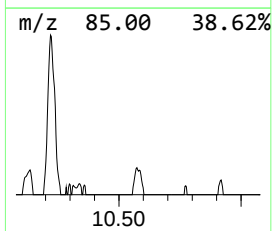
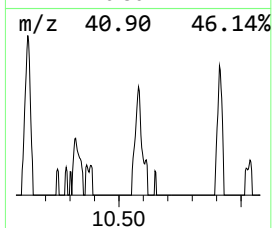
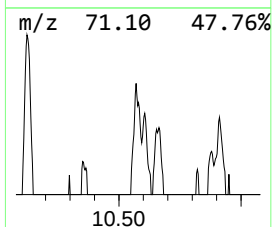
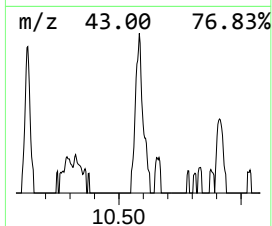
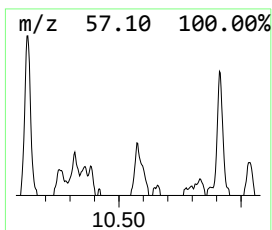
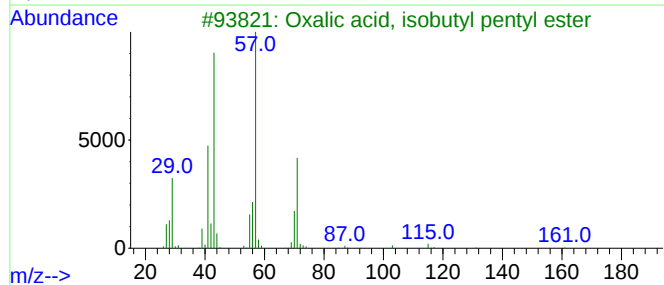
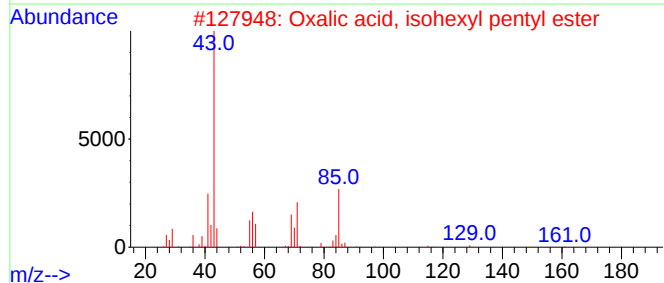
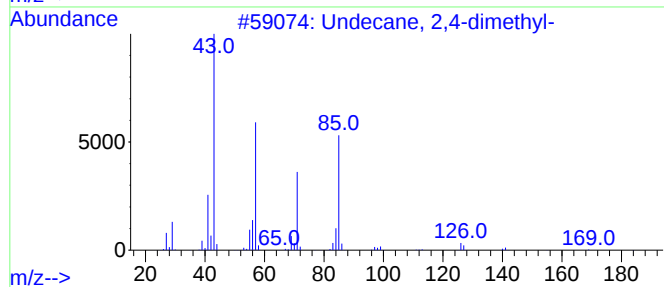
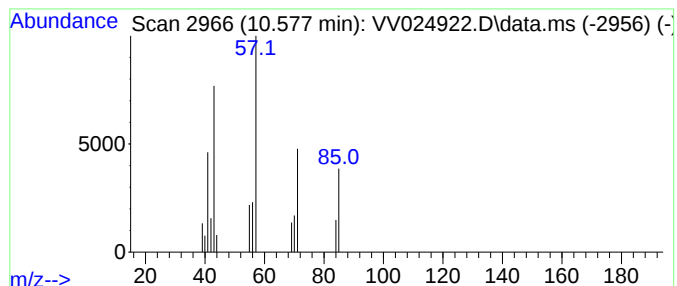
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Quant Title : VOC Analysis

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.577	2.68 ug/L	9706	1,4-Dichlorobenzene-d4	11.252

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 2,4-dimethyl-	184	C13H28	017312-80-0	78
2			Oxalic acid, isohexyl pentyl ester	244	C13H24O4	1000309-32-8	64
3			Oxalic acid, isobutyl pentyl ester	216	C11H20O4	1000309-37-0	50
4			Octane	114	C8H18	000111-65-9	45
5			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV031022\
Data File : VV024922.D
Acq On : 10 Mar 2022 17:43
Operator : SY/MD
Sample : N1816-20ME
Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBSE5ME

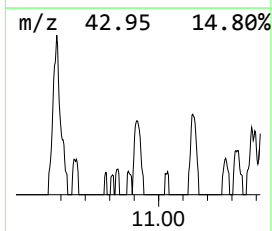
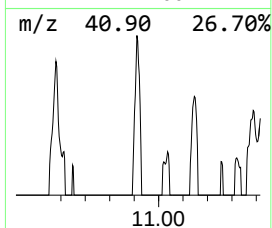
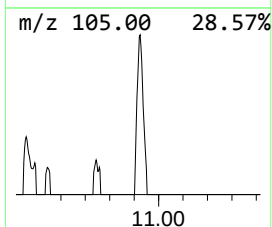
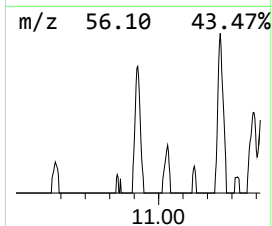
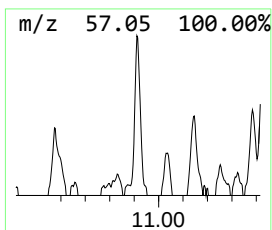
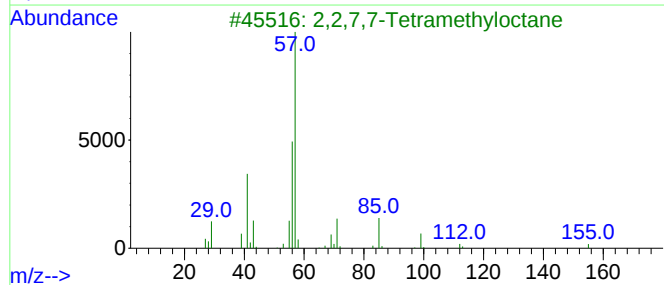
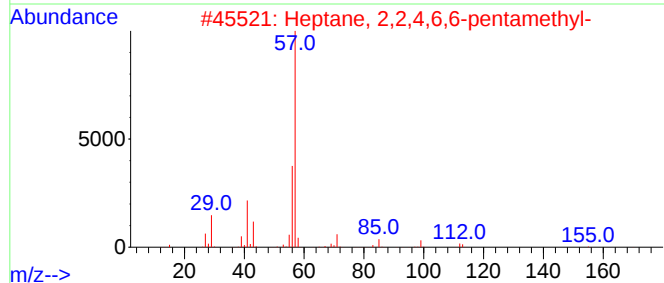
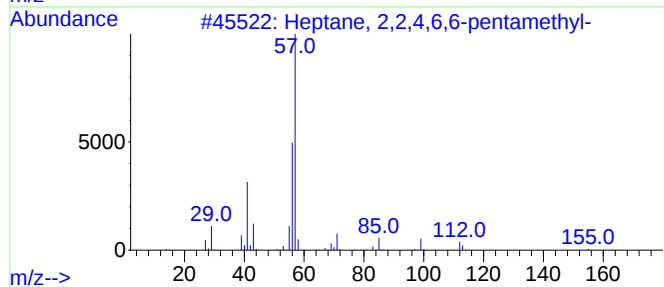
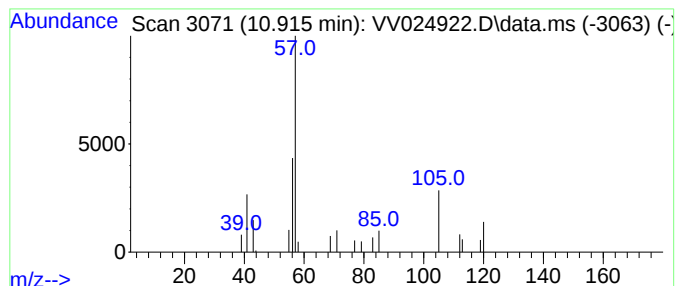
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Quant Title : VOC Analysis

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.915	3.14 ug/L	11378	1,4-Dichlorobenzene-d4	11.252

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	53
2			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	53
3			2,2,7,7-Tetramethyloctane	170	C12H26	001071-31-4	47
4			Dodecane, 2,2,11,11-tetramethyl-	226	C16H34	127204-12-0	40
5			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	40



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV031022\
Data File : VV024922.D
Acq On : 10 Mar 2022 17:43
Operator : SY/MD
Sample : N1816-20ME
Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBSE5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022822WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Furan, tetrahyd...	5.342	4.1	ug/L	11673	1	5.619	142541	50.0
unknown-01	5.902	35.5	ug/L	101338	1	5.619	142541	50.0
(DEL) Alkane: S...	10.127	3.8	ug/L	13712	3	11.252	181149	50.0
(DEL) Alkane: S...	10.577	2.7	ug/L	9706	3	11.252	181149	50.0
(DEL) Alkane: S...	10.915	3.1	ug/L	11378	3	11.252	181149	50.0