

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
 Data File : VU043731.D
 Acq On : 14 May 2021 04:15
 Operator : SY/MD
 Sample : M2350-02
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BG6L5

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\SFAMULM051421WMA.M

Title : VOC Analysis

Signal : TIC: VU043731.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.363	3	7	11	rBV3	5266	4964	0.02%	0.009%
2	1.604	73	82	97	rBV2	271163	315515	1.35%	0.557%
3	1.912	170	178	197	rVB2	170229	267948	1.15%	0.473%
4	2.578	370	385	400	rBV3	626997	1240844	5.32%	2.189%
5	2.764	430	443	461	rBV	28280	61426	0.26%	0.108%
6	2.999	513	516	520	rBV4	582	402	0.00%	0.001%
7	3.051	524	532	539	rBV5	2113	3786	0.02%	0.007%
8	3.182	557	573	599	rBV2	71353	171555	0.74%	0.303%
9	3.359	616	628	642	rVB2	8645	16781	0.07%	0.030%
10	3.552	682	688	693	rBV3	322	489	0.00%	0.001%
11	3.584	693	698	700	rBV2	508	512	0.00%	0.001%
12	3.877	769	789	812	rBV	2250223	5354727	22.96%	9.447%
13	4.002	815	828	847	rVB	65326	171239	0.73%	0.302%
14	4.205	888	891	893	rBV3	988	667	0.00%	0.001%
15	4.536	984	994	996	rBV7	2072	2793	0.01%	0.005%
16	4.626	1008	1022	1032	rBV	200362	475283	2.04%	0.838%
17	4.809	1074	1079	1093	rVB3	7006	14397	0.06%	0.025%
18	5.073	1143	1161	1183	rBV	307921	676885	2.90%	1.194%
19	5.327	1218	1240	1271	rBV	10401195	23324063	100.00%	41.148%
20	5.732	1346	1366	1400	rVB2	666499	1830944	7.85%	3.230%
21	6.256	1510	1529	1551	rBV	516245	958615	4.11%	1.691%
22	6.507	1603	1607	1608	rBV2	786	508	0.00%	0.001%
23	6.552	1609	1621	1623	rBV6	7936	13106	0.06%	0.023%
24	6.697	1649	1666	1683	rBV	405642	789858	3.39%	1.393%
25	6.922	1719	1736	1768	rBV	306071	605140	2.59%	1.068%
26	7.034	1768	1771	1773	rBV3	758	565	0.00%	0.001%
27	7.124	1796	1799	1804	rVB4	529	461	0.00%	0.001%
28	7.182	1804	1817	1827	rVB8	1701	3694	0.02%	0.007%
29	7.256	1832	1840	1851	rVB4	3234	5523	0.02%	0.010%
30	7.346	1854	1868	1894	rBV	217653	416424	1.79%	0.735%
31	7.523	1908	1923	1931	rBV	303321	555409	2.38%	0.980%
32	7.571	1931	1938	1964	rVB	233770	414046	1.78%	0.730%
33	7.719	1970	1984	2003	rVB	277565	517750	2.22%	0.913%
34	7.906	2028	2042	2055	rBV	827671	1405366	6.03%	2.479%
35	7.976	2056	2064	2075	rVB	29666	51987	0.22%	0.092%
36	8.185	2117	2129	2143	rBV	154016	253481	1.09%	0.447%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
 Title : VOC Analysis

37	8.385	2181	2191	2192	rBV3	4593	4882	0.02%	0.009%
38	8.494	2216	2225	2238	rVB5	3374	6419	0.03%	0.011%
39	8.562	2238	2246	2253	rVB4	4969	7192	0.03%	0.013%
40	8.639	2256	2270	2298	rBV	558709	991040	4.25%	1.748%
41	8.809	2320	2323	2326	rBV4	842	620	0.00%	0.001%
42	8.848	2330	2335	2345	rVB6	2800	4092	0.02%	0.007%
43	8.928	2352	2360	2369	rVB9	945	1866	0.01%	0.003%
44	9.047	2391	2397	2406	rVB6	3276	4705	0.02%	0.008%
45	9.137	2421	2425	2433	rBV3	1198	1427	0.01%	0.003%
46	9.192	2435	2442	2447	rVV6	1004	1329	0.01%	0.002%
47	9.224	2448	2452	2458	rVB3	1588	1627	0.01%	0.003%
48	9.320	2474	2482	2500	rVB2	12488	22619	0.10%	0.040%
49	9.423	2500	2514	2536	rBV	716598	1333504	5.72%	2.353%
50	9.523	2537	2545	2555	rVB3	26398	43593	0.19%	0.077%
51	9.697	2590	2599	2612	rVV4	5543	11285	0.05%	0.020%
52	9.764	2612	2620	2633	rVB3	3571	5714	0.02%	0.010%
53	9.996	2684	2692	2701	rVB6	1738	2585	0.01%	0.005%
54	10.054	2703	2710	2715	rBV7	1279	2130	0.01%	0.004%
55	10.108	2719	2727	2739	rVB4	7636	13881	0.06%	0.024%
56	10.263	2760	2775	2795	rBV	2356999	4116858	17.65%	7.263%
57	10.549	2856	2864	2874	rBV2	71286	122348	0.52%	0.216%
58	10.761	2916	2930	2942	rBV	558507	940763	4.03%	1.660%
59	10.896	2958	2972	2981	rBV9	52177	146434	0.63%	0.258%
60	10.944	2982	2987	2995	rVB2	57350	76684	0.33%	0.135%
61	10.992	2995	3002	3003	rBV	27499	25869	0.11%	0.046%
62	11.037	3004	3016	3035	rVB	3173035	5274694	22.61%	9.306%
63	11.124	3035	3043	3051	rBV	100211	145407	0.62%	0.257%
64	11.198	3060	3066	3073	rVV	72217	94806	0.41%	0.167%
65	11.243	3074	3080	3089	rVB	55169	79369	0.34%	0.140%
66	11.298	3090	3097	3103	rBV	17459	24388	0.10%	0.043%
67	11.340	3103	3110	3121	rVB2	39867	57523	0.25%	0.101%
68	11.484	3142	3155	3166	rBV5	15456	34749	0.15%	0.061%
69	11.574	3177	3183	3190	rVB6	7204	9896	0.04%	0.017%
70	11.642	3190	3204	3216	rBV6	18470	41576	0.18%	0.073%
71	11.716	3217	3227	3237	rBV5	26639	43774	0.19%	0.077%
72	11.819	3244	3259	3275	rBV	736948	1177978	5.05%	2.078%
73	11.906	3278	3286	3295	rVB3	23096	33656	0.14%	0.059%
74	12.102	3331	3347	3359	rBV2	141284	230118	0.99%	0.406%
75	12.198	3364	3377	3394	rVV	797032	1337178	5.73%	2.359%
76	12.426	3443	3448	3455	rVB6	3149	3828	0.02%	0.007%

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Peak Location: TOP

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 Title : VOC Analysis

77	12.497	3463	3470	3477	rBV8	4598	7325	0.03%	0.013%
78	12.561	3483	3490	3499	rVB7	7087	10885	0.05%	0.019%
79	12.616	3499	3507	3514	rBV3	10230	14183	0.06%	0.025%
80	12.661	3514	3521	3524	rBV7	5393	6444	0.03%	0.011%
81	12.870	3576	3586	3597	rVB2	40518	62704	0.27%	0.111%
82	12.951	3598	3611	3628	rVB7	25775	58990	0.25%	0.104%
83	13.124	3658	3665	3668	rBV8	3075	4176	0.02%	0.007%
84	13.156	3670	3675	3683	rVB5	6865	8914	0.04%	0.016%
85	13.262	3699	3708	3723	rBV8	17878	38505	0.17%	0.068%
86	13.407	3745	3753	3758	rBV5	636	1118	0.00%	0.002%
87	13.455	3762	3768	3777	rVB5	3227	5433	0.02%	0.010%
88	13.533	3786	3792	3799	rVB6	1850	2693	0.01%	0.005%
89	13.729	3845	3853	3861	rBV7	3135	5377	0.02%	0.009%
90	13.790	3865	3872	3880	rBV5	2084	3014	0.01%	0.005%
91	13.848	3884	3890	3896	rVB6	2187	2512	0.01%	0.004%
92	13.883	3897	3901	3903	rBV4	998	834	0.00%	0.001%
93	13.915	3904	3911	3912	rBV5	3594	3488	0.01%	0.006%
94	14.176	3984	3992	3999	rBV7	9656	13228	0.06%	0.023%
95	14.288	4023	4027	4031	rBV5	1901	2087	0.01%	0.004%
96	14.770	4170	4177	4185	rBV6	6550	8789	0.04%	0.016%
97	14.815	4187	4191	4197	rVB5	1171	1120	0.00%	0.002%
98	14.886	4208	4213	4220	rVB7	3357	4458	0.02%	0.008%
99	15.031	4252	4258	4268	rVB7	2343	3867	0.02%	0.007%
100	16.899	4833	4839	4845	rBV4	6207	7200	0.03%	0.013%

Sum of corrected areas: 56682903

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ClientSampleId :
BG6L5

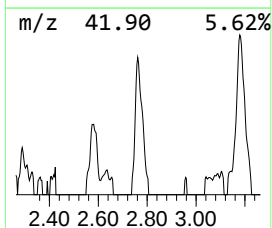
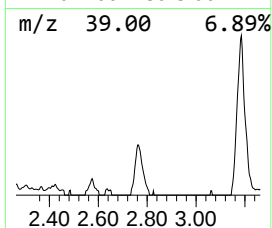
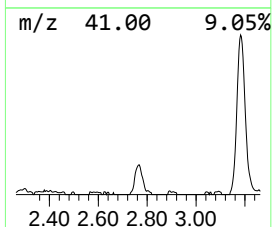
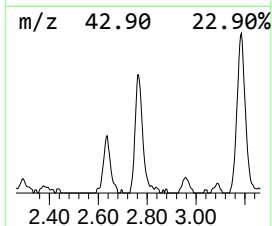
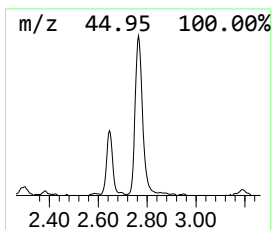
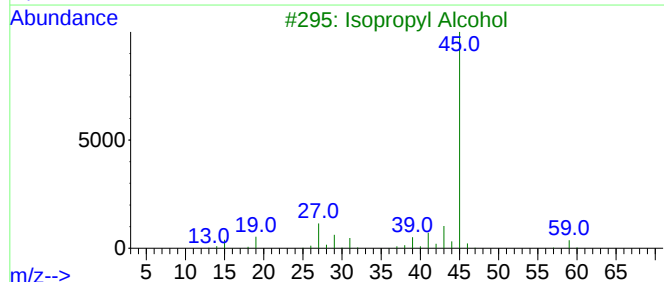
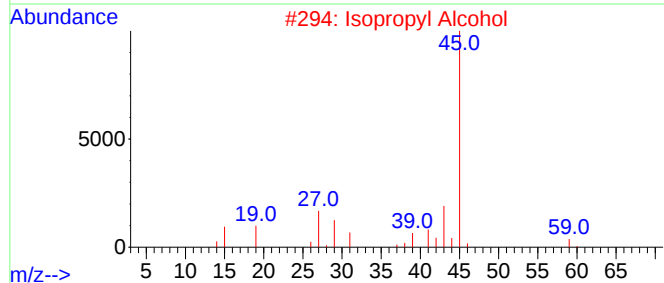
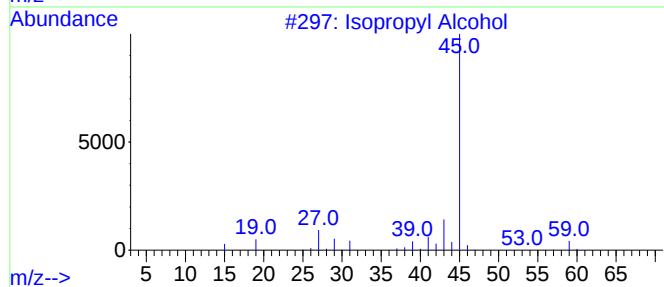
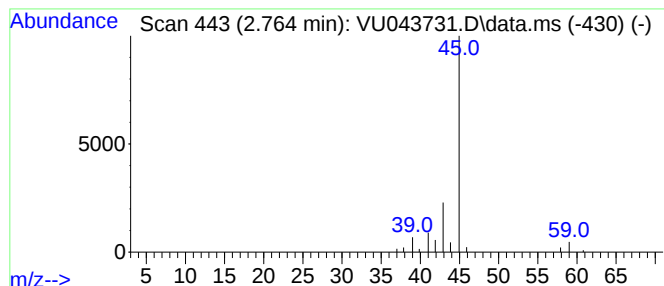
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.764	3.20 ug/L	61426	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	74
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	64
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5			Ethylamine	45	C2H7N	000075-04-7	5



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Sample : M2350-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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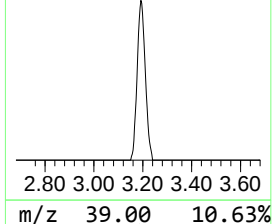
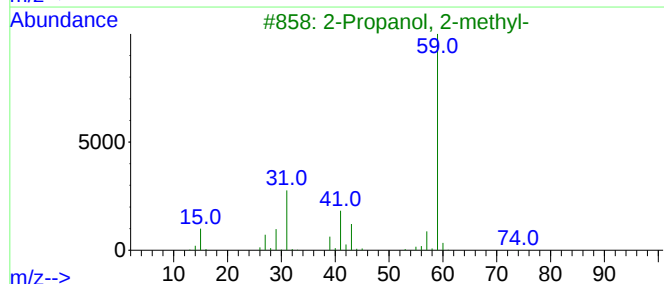
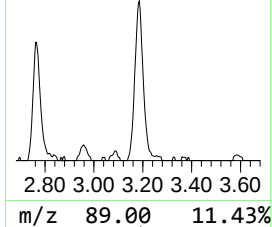
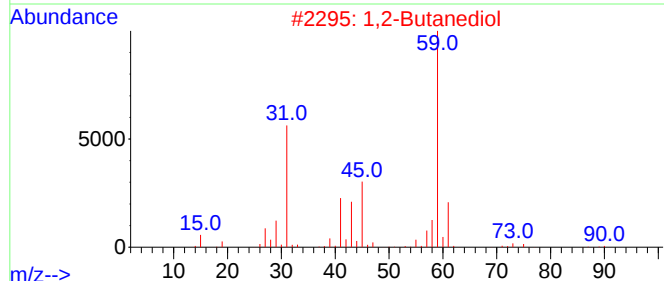
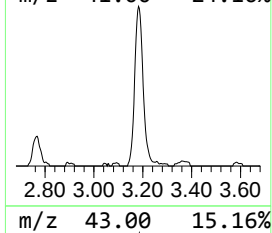
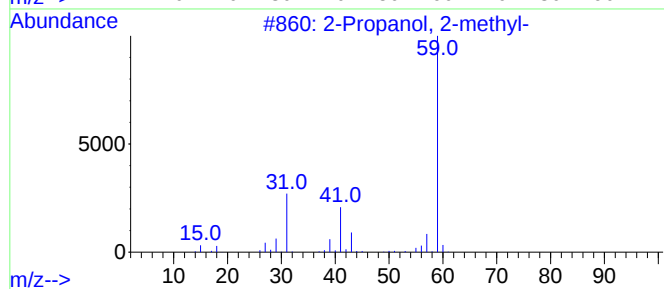
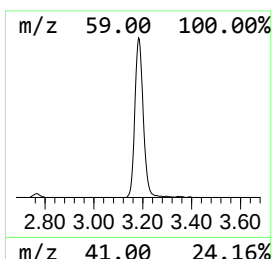
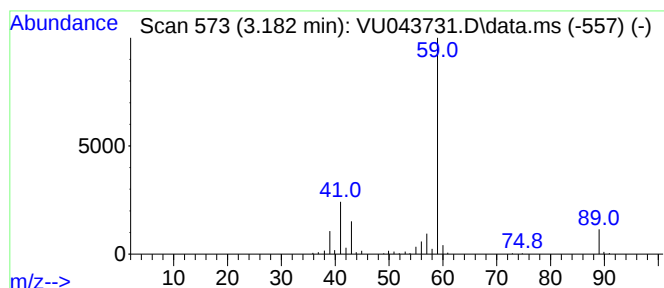
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 2-Propanol, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.182	8.95 ug/L	171555	1,4-Difluorobenzene	6.256

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	64
2		1,2-Butanediol	90	C4H10O2	000584-03-2	64
3		2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	39
4		1,2-Butanediol	90	C4H10O2	000584-03-2	38
5		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	38



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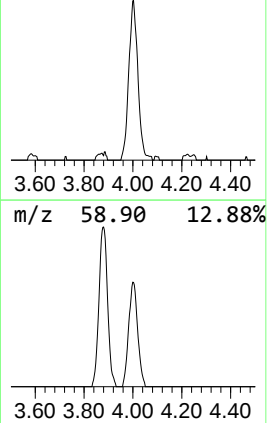
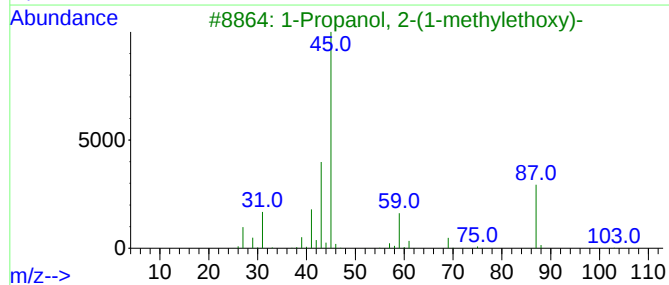
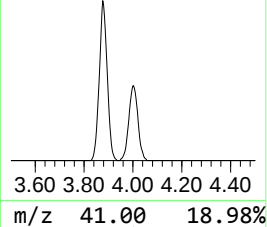
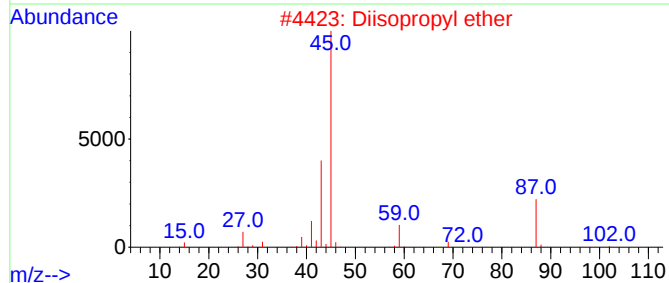
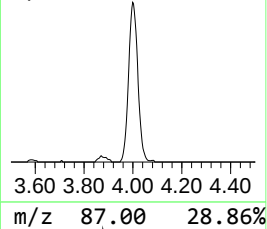
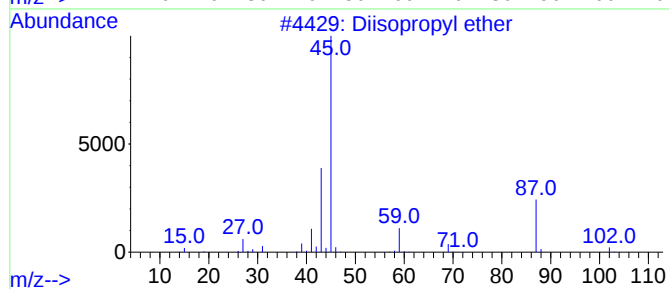
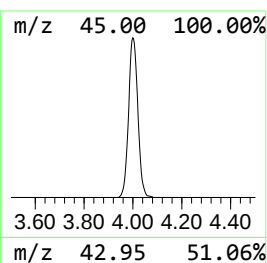
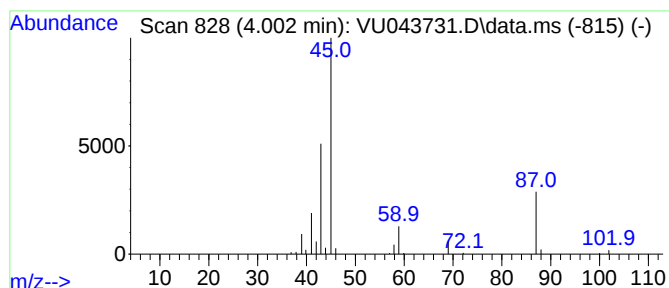
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Diisopropyl ether Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.002	8.93 ug/L	171239	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diisopropyl ether	102	C6H14O	000108-20-3	86
2			Diisopropyl ether	102	C6H14O	000108-20-3	83
3			1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	78
4			Diisopropyl ether	102	C6H14O	000108-20-3	78
5			1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	72



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Instrument :
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ClientSampleId :
BG6L5

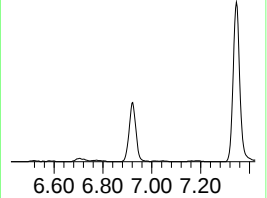
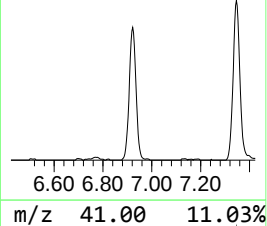
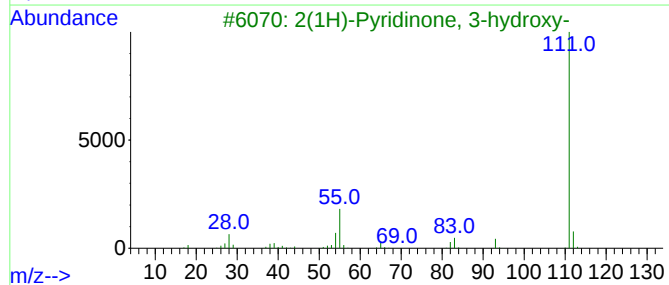
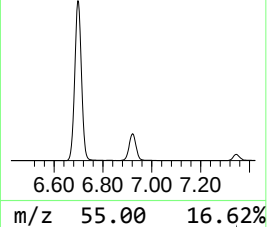
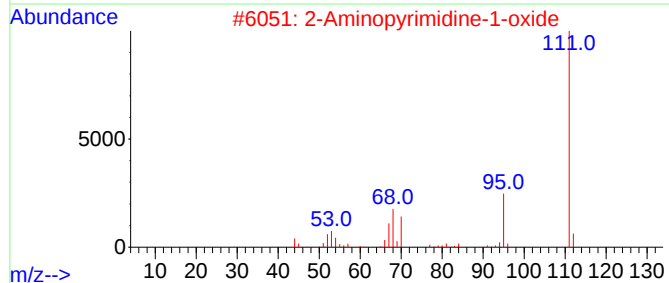
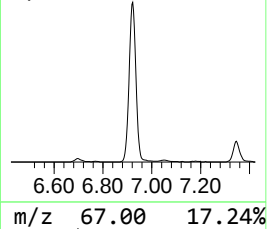
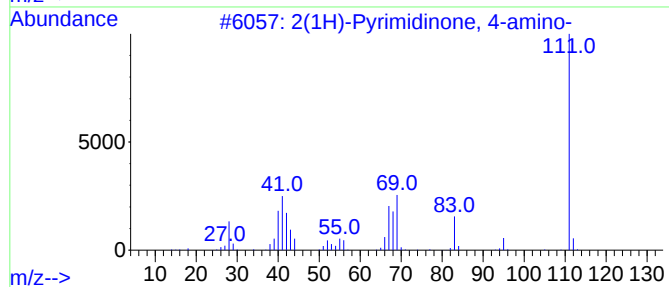
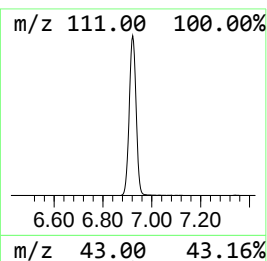
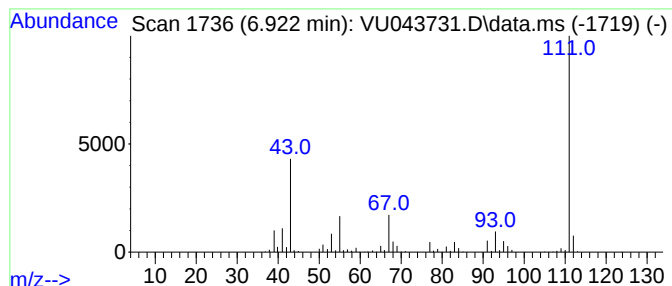
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Quant Title : VOC Analysis

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

Peak Number 4 2(1H)-Pyrimidinone, 4-amino- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.922	31.56 ug/L	605140	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	64		
2	2-Aminopyrimidine-1-oxide	111	C4H5N3O	035034-15-2	50		
3	2(1H)-Pyridinone, 3-hydroxy-	111	C5H5N2O2	016867-04-2	45		
4	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	39		
5	2(1H)-Pyrimidinone, 4-amino-	111	C4H5N3O	000071-30-7	39		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043731.D
Acq On : 14 May 2021 04:15
Operator : SY/MD
Sample : M2350-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG6L5

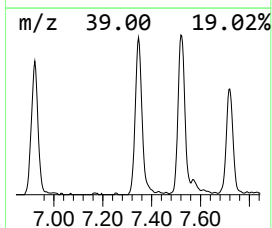
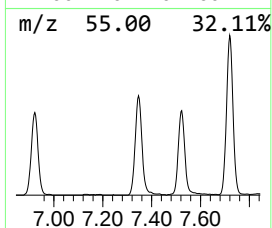
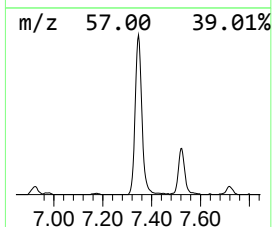
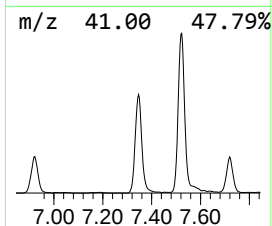
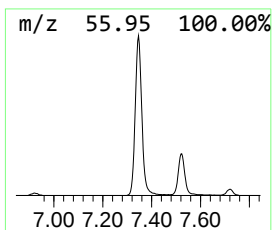
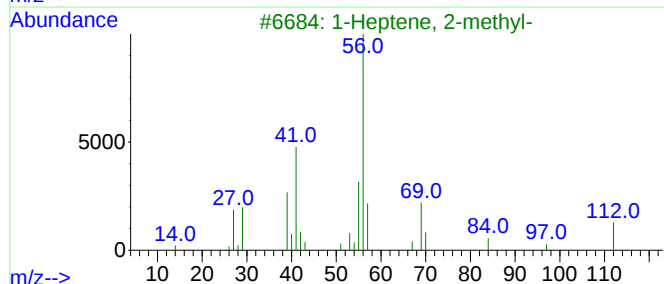
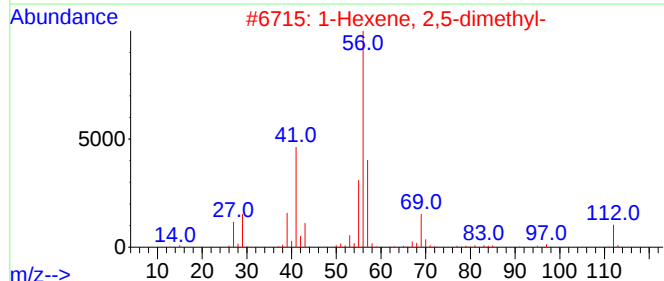
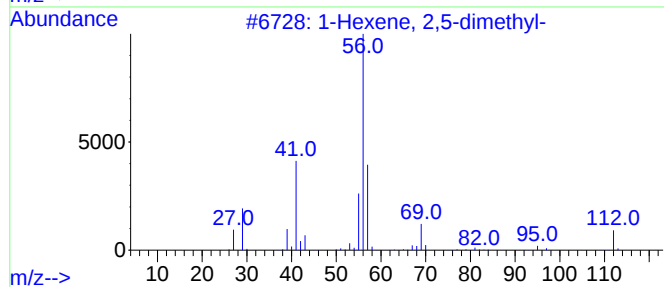
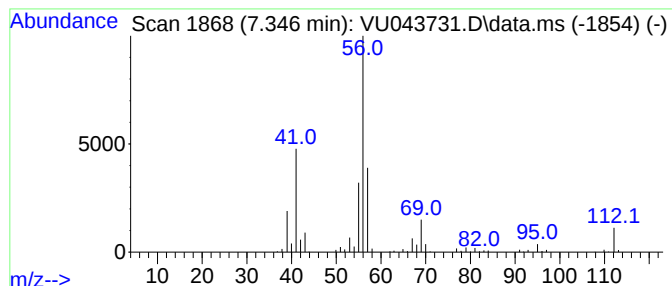
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Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.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.
7.346	21.72 ug/L	416424	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	91
2			1-Hexene, 2,5-dimethyl-	112	C8H16	006975-92-4	90
3			1-Heptene, 2-methyl-	112	C8H16	015870-10-7	72
4			2,4-Dimethyl-1-hexene	112	C8H16	016746-87-5	59
5			Cyclopentanone, 2,2-dimethyl-	112	C7H12O	004541-32-6	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043731.D
Acq On : 14 May 2021 04:15
Operator : SY/MD
Sample : M2350-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG6L5

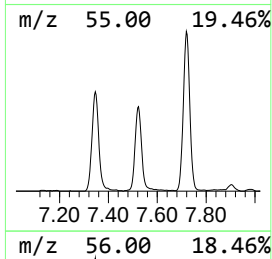
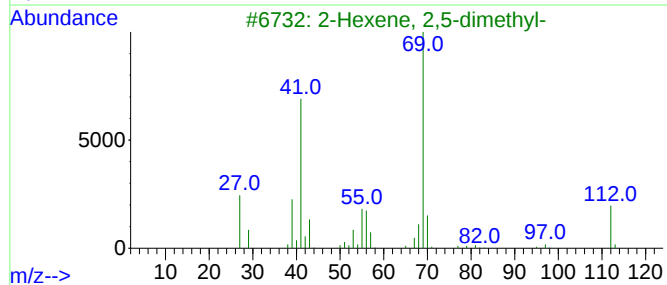
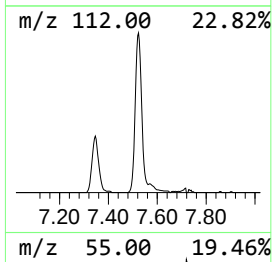
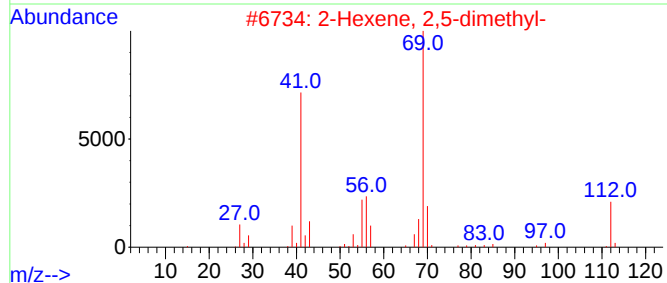
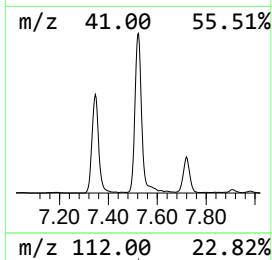
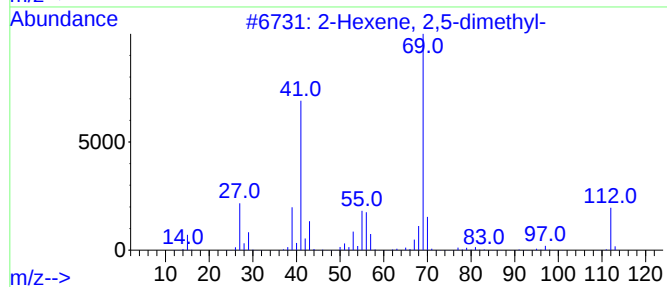
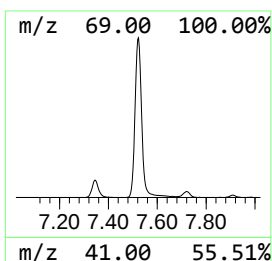
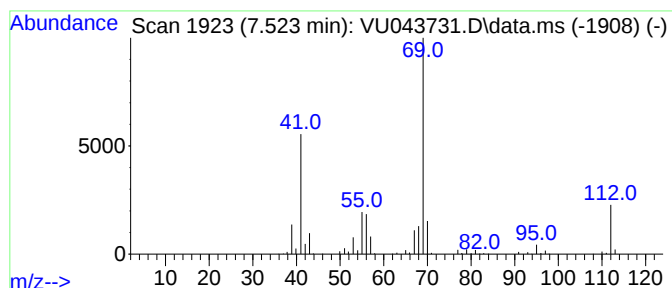
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Quant Title : VOC Analysis

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

Peak Number 6 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.523	28.97 ug/L	555409	1,4-Difluorobenzene	6.256

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	90	
2	2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	90	
3	2-Hexene, 2,5-dimethyl-	112	C8H16	003404-78-2	90	
4	3-Hexene, 2,5-dimethyl-, (E)-	112	C8H16	000692-70-6	78	
5	3-Hexene, 2,5-dimethyl-	112	C8H16	015910-22-2	72	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043731.D
Acq On : 14 May 2021 04:15
Operator : SY/MD
Sample : M2350-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG6L5

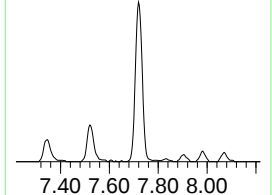
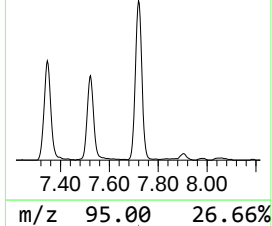
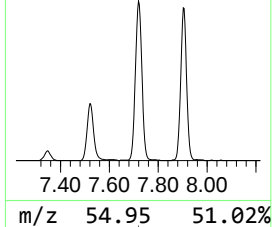
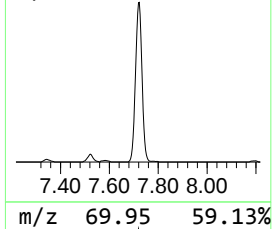
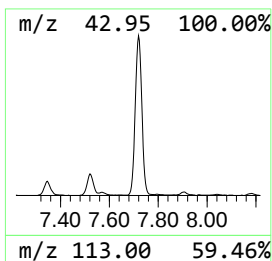
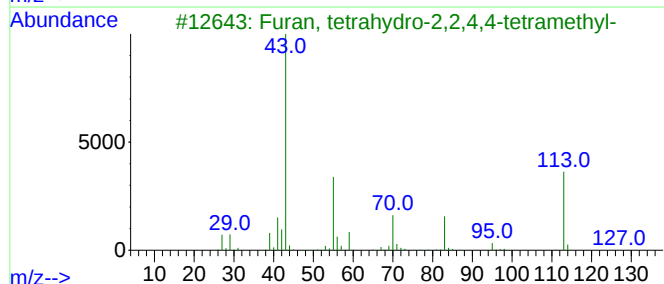
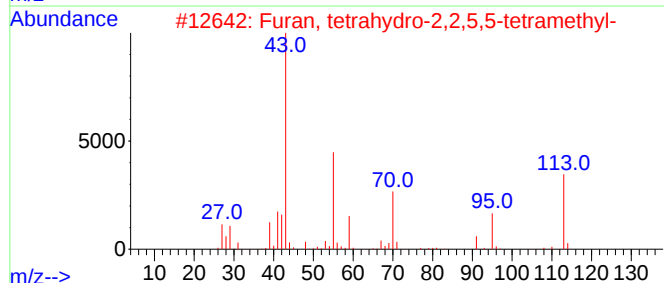
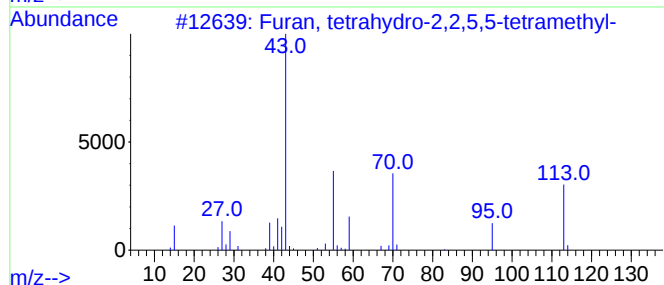
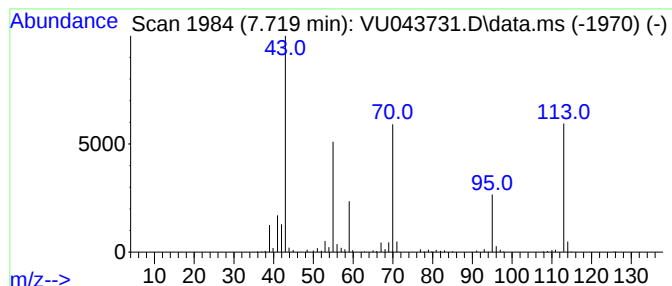
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Quant Title : VOC Analysis

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

Peak Number 8 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.719	27.01 ug/L	517750	1,4-Difluorobenzene	6.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	83
2			Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	74
3			Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	53
4			4-Piperidinone, 1-methyl-	113	C6H11NO	001445-73-4	50
5			Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043731.D
Acq On : 14 May 2021 04:15
Operator : SY/MD
Sample : M2350-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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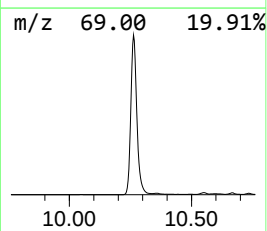
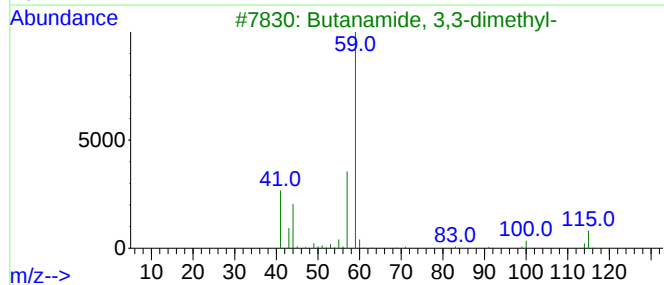
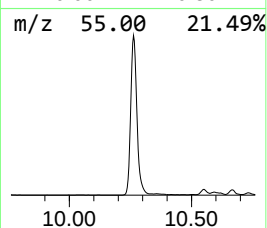
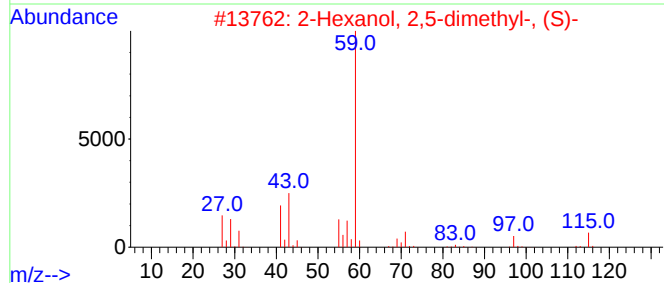
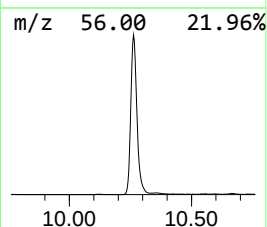
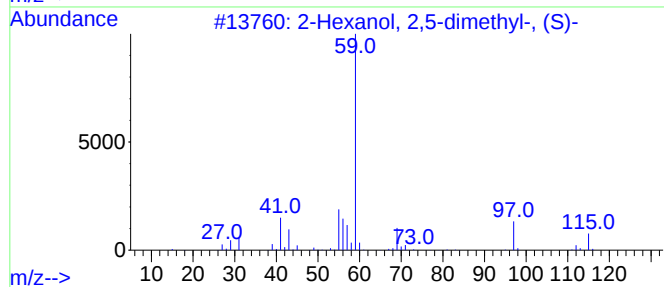
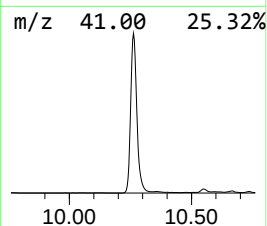
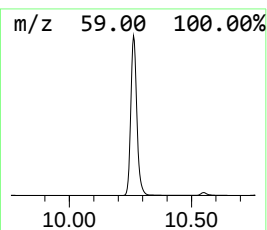
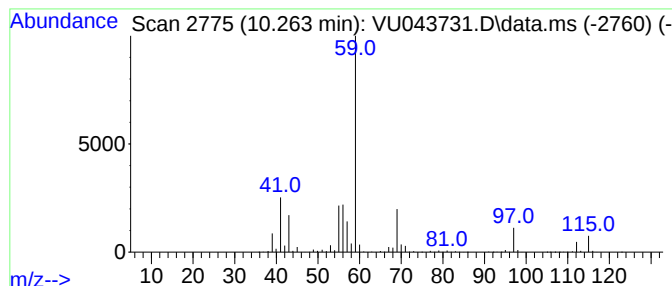
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Quant Title : VOC Analysis

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

Peak Number 9 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.262	154.36 ug/L	4116860	Chlorobenzene-d5	9.423

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	78
2			2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	64
3			Butanamide, 3,3-dimethyl-	115	C6H13NO	000926-04-5	47
4			Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	45
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043731.D
Acq On : 14 May 2021 04:15
Operator : SY/MD
Sample : M2350-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG6L5

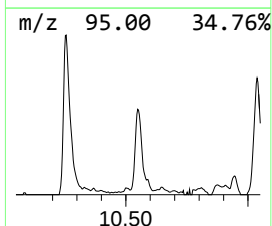
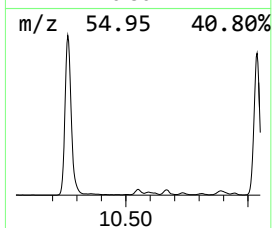
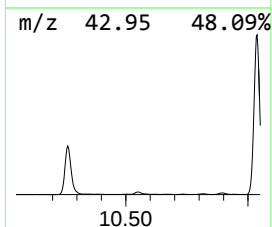
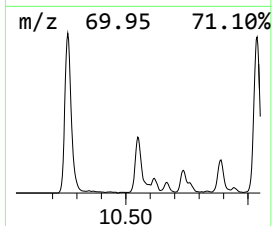
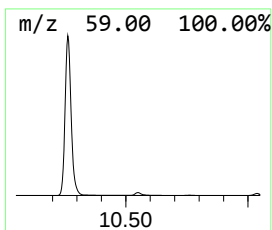
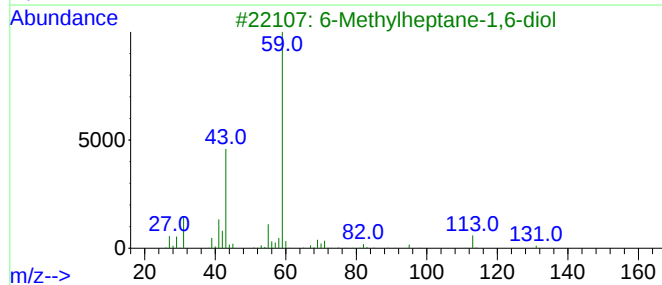
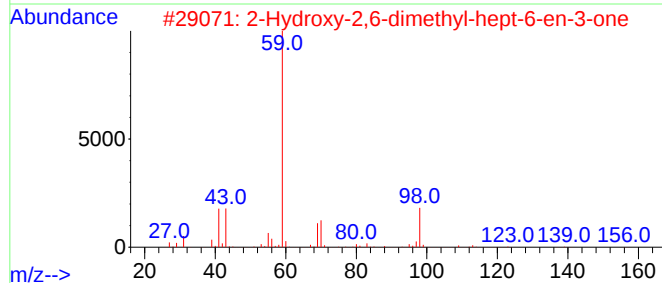
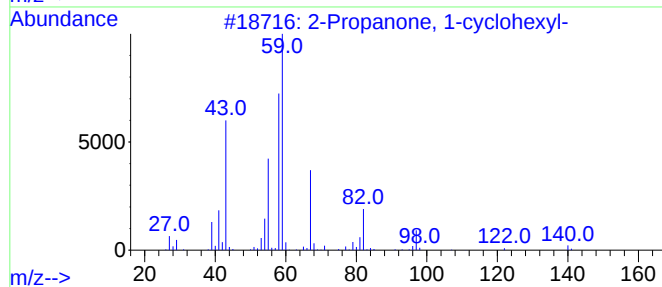
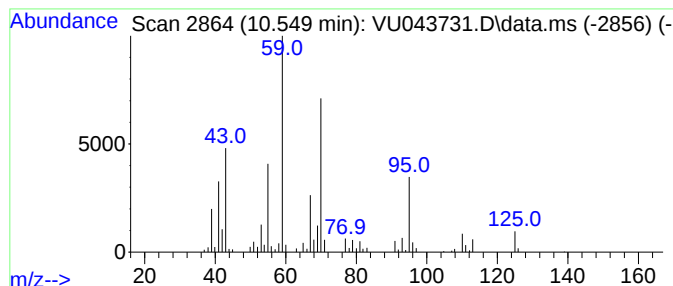
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Quant Title : VOC Analysis

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

Peak Number 10 unknown-01 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.549	4.59 ug/L	122348	Chlorobenzene-d5	9.423

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propanone, 1-cyclohexyl-	140	C9H16O	000103-78-6	38
2			2-Hydroxy-2,6-dimethyl-hept-6-en...	156	C9H16O2	001068-82-2	38
3			6-Methylheptane-1,6-diol	146	C8H18O2	005392-57-4	35
4			Oxetane, 2,2,3-trimethyl-	100	C6H12O	023120-43-6	33
5			Heptane, 1-ethoxy-	144	C9H20O	001969-43-3	25



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043731.D
Acq On : 14 May 2021 04:15
Operator : SY/MD
Sample : M2350-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

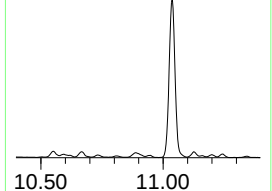
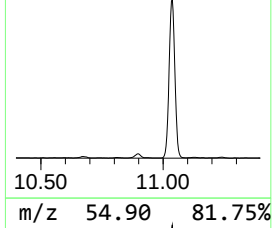
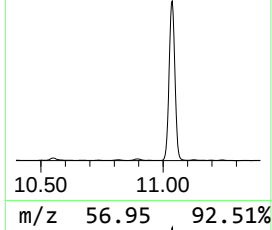
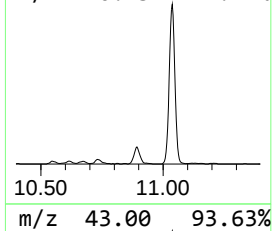
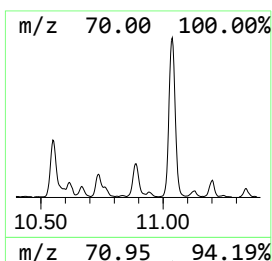
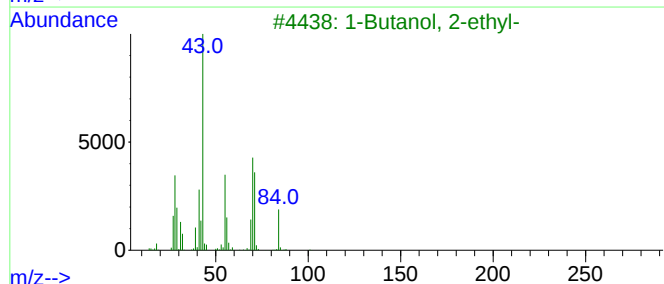
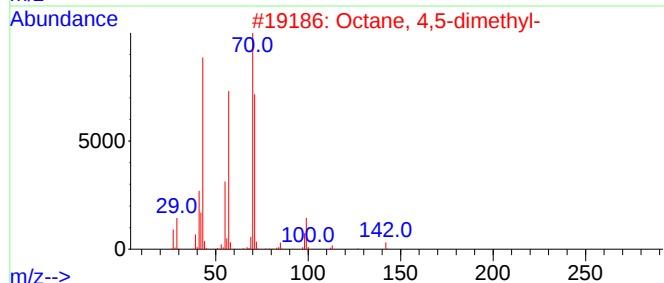
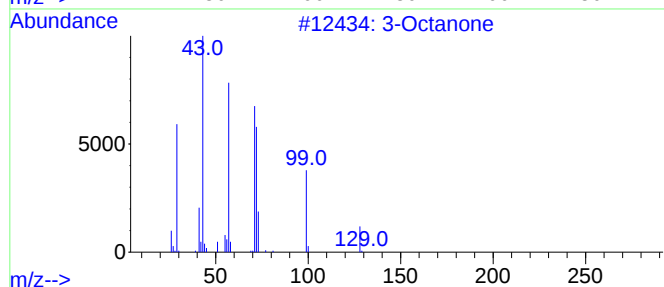
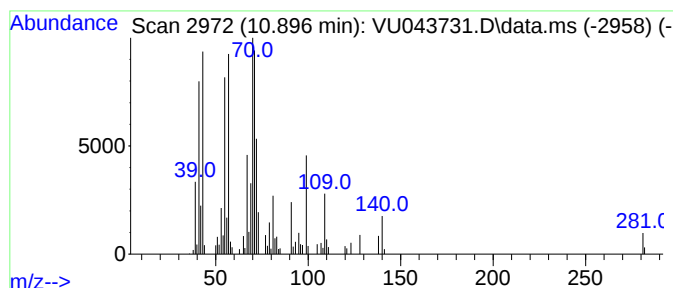
Instrument :
MSVOA_U
ClientSampleId :
BG6L5

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Quant Title : VOC Analysis

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

Peak Number 11 unknown-02 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.896	6.22 ug/L	146434	1,4-Dichlorobenzene-d4	11.819	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Octanone	128	C8H16O	000106-68-3	38
2	Octane, 4,5-dimethyl-	142	C10H22	015869-96-2	38
3	1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	35
4	3,6-Dimethyl-4-octanone	156	C10H20O	034645-03-9	35
5	3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043731.D
Acq On : 14 May 2021 04:15
Operator : SY/MD
Sample : M2350-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG6L5

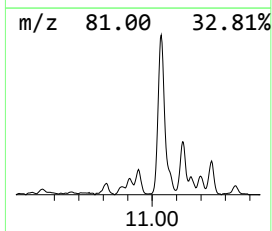
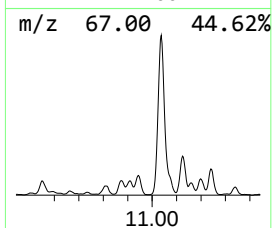
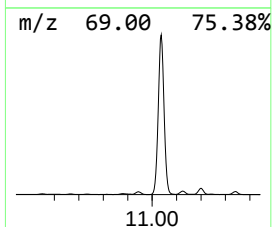
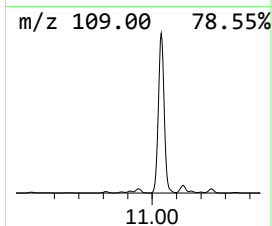
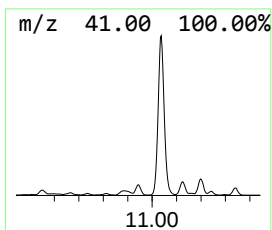
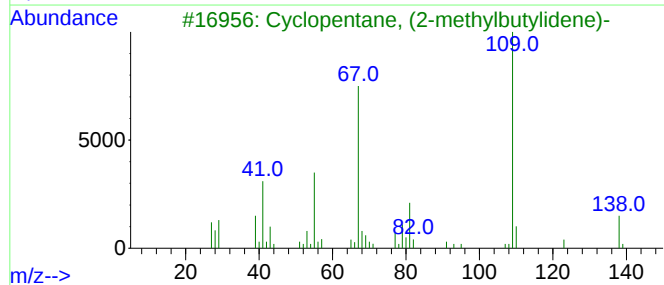
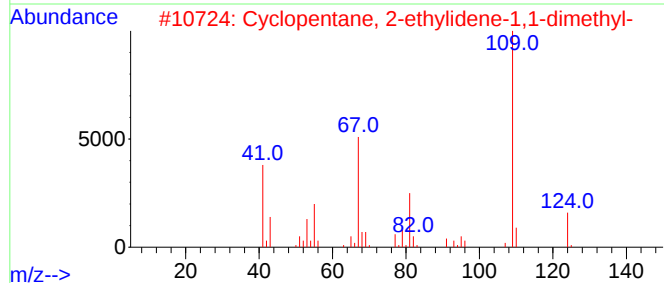
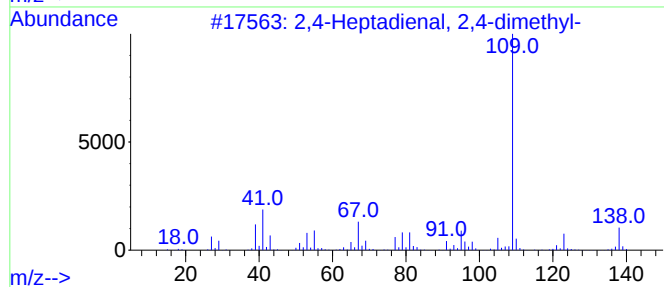
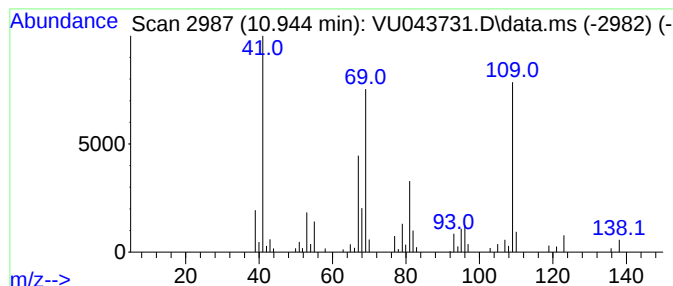
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Quant Title : VOC Analysis

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

Peak Number 12 unknown-03 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.944	3.25 ug/L	76684	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Heptadienal, 2,4-dimethyl-	138	C9H14O	042452-48-2	43
2			Cyclopentane, 2-ethylidene-1,1-d...	124	C9H16	056324-66-4	43
3			Cyclopentane, (2-methylbutylidene)-	138	C10H18	053366-54-4	38
4			Cyclohexanol, 3,3,5-trimethyl-	142	C9H18O	000116-02-9	38
5			3-Heptyne, 5-ethyl-5-methyl-	138	C10H18	061228-10-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043731.D
Acq On : 14 May 2021 04:15
Operator : SY/MD
Sample : M2350-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG6L5

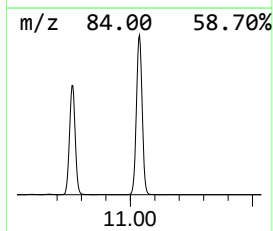
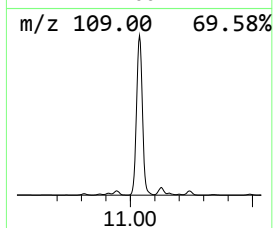
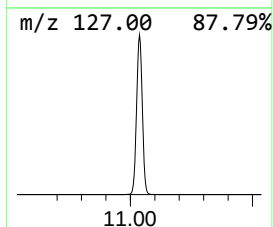
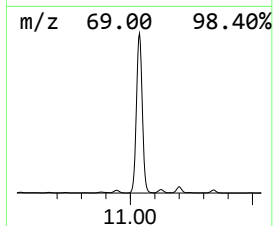
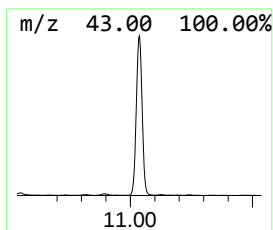
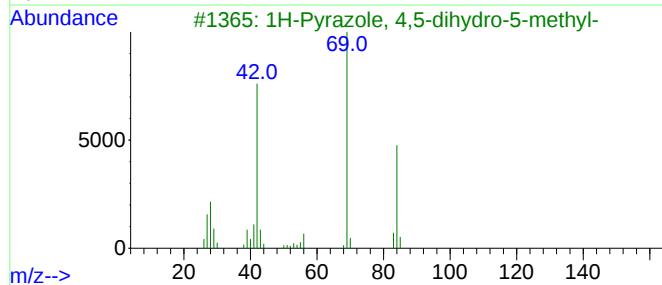
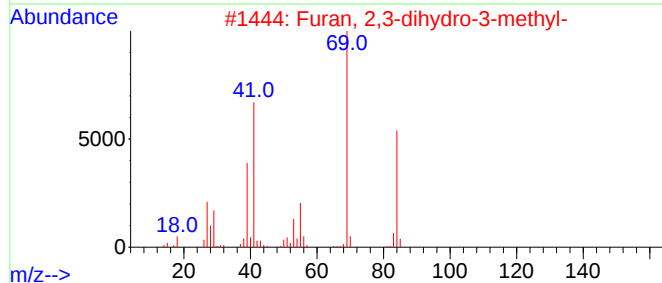
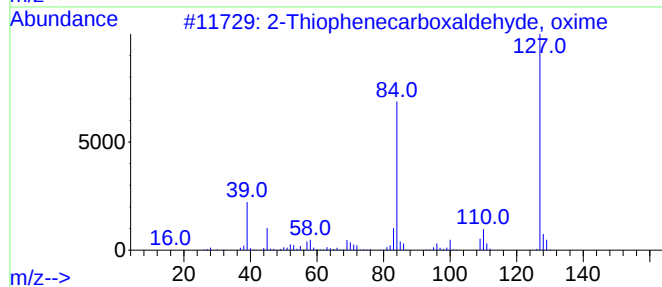
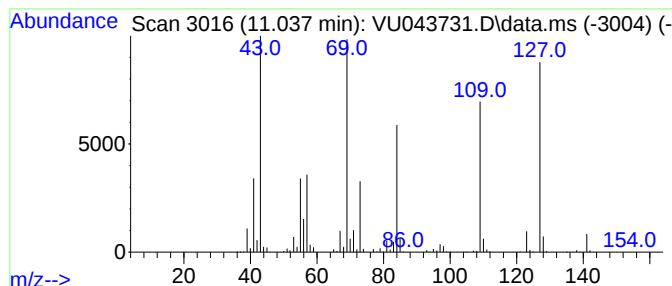
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Quant Title : VOC Analysis

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

Peak Number 13 unknown-04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.037	223.89 ug/L	5274690	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Thiophenecarboxaldehyde, oxime	127	C5H5NOS	029683-84-9	35
2			Furan, 2,3-dihydro-3-methyl-	84	C5H8O	001708-27-6	30
3			1H-Pyrazole, 4,5-dihydro-5-methyl-	84	C4H8N2	001568-20-3	27
4			Pentane, 2-chloro-4-methyl-	120	C6H13Cl	025346-32-1	27
5			Pentane, 3-methylene-	84	C6H12	000760-21-4	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043731.D
Acq On : 14 May 2021 04:15
Operator : SY/MD
Sample : M2350-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG6L5

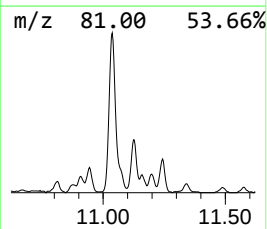
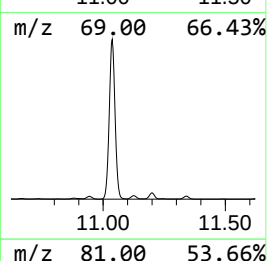
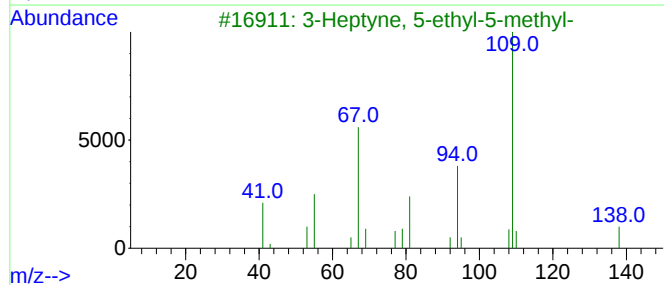
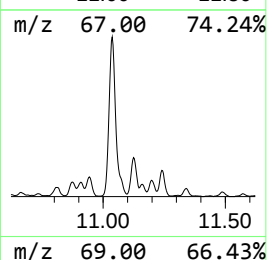
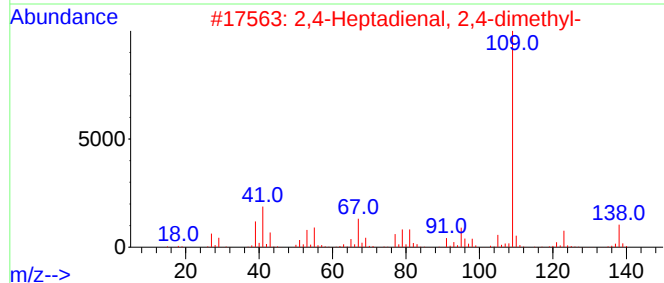
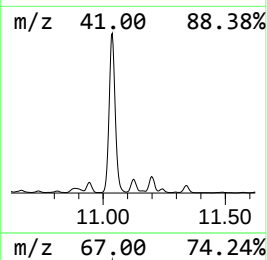
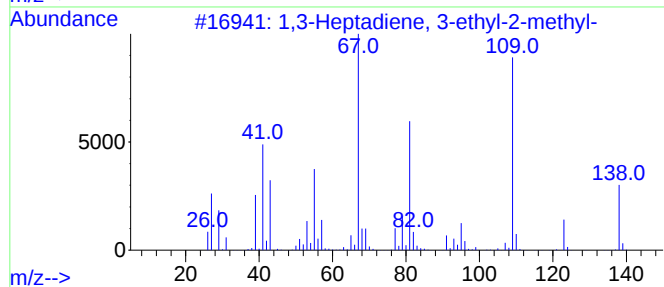
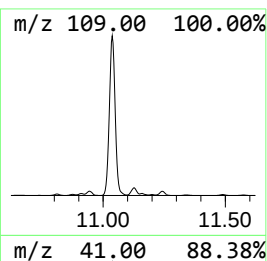
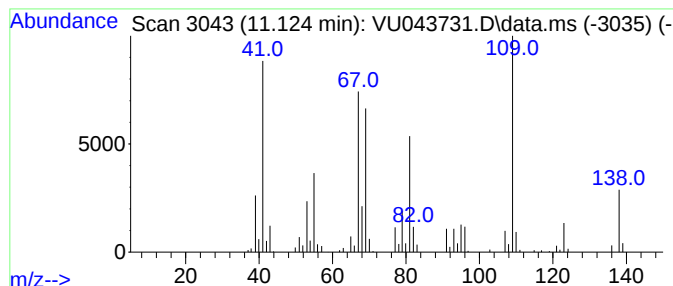
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Quant Title : VOC Analysis

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

Peak Number 14 1,3-Heptadiene, 3-ethyl-2-m... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.124	6.17 ug/L	145407	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Heptadiene, 3-ethyl-2-methyl-	138	C10H18	061142-35-6	74		
2	2,4-Heptadienal, 2,4-dimethyl-	138	C9H14O	042452-48-2	72		
3	3-Heptyne, 5-ethyl-5-methyl-	138	C10H18	061228-10-2	64		
4	4-Octyne	110	C8H14	001942-45-6	64		
5	Cyclopentane, 2-ethylidene-1,1-d...	124	C9H16	056324-66-4	59		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043731.D
Acq On : 14 May 2021 04:15
Operator : SY/MD
Sample : M2350-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG6L5

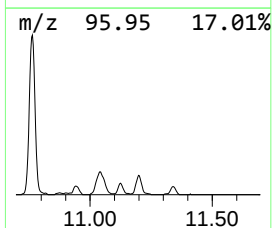
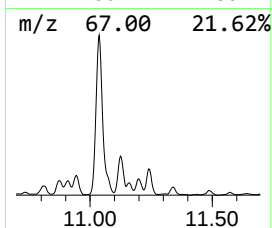
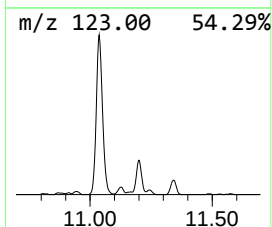
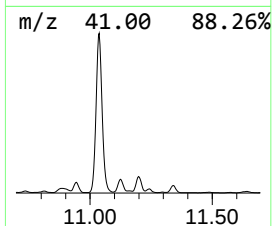
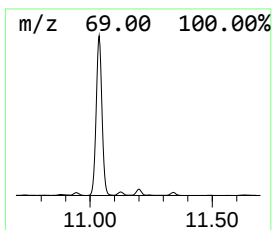
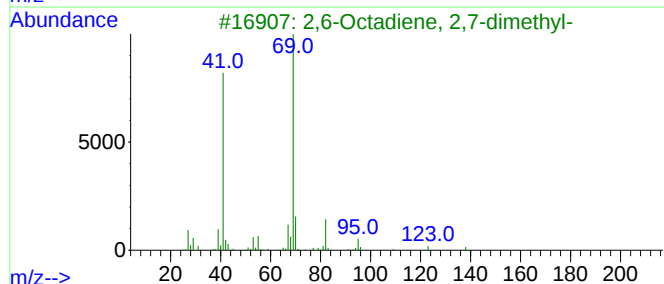
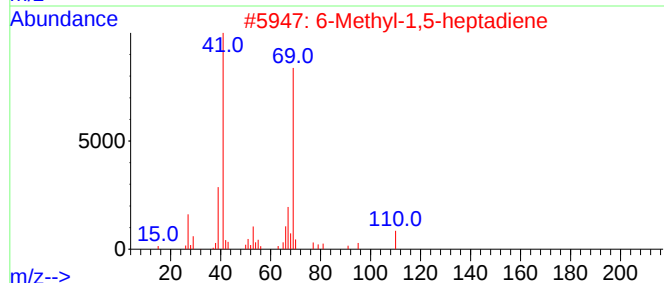
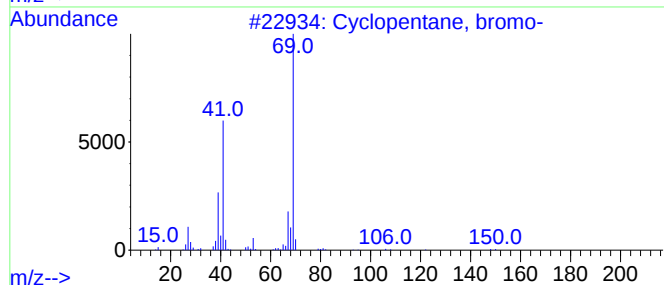
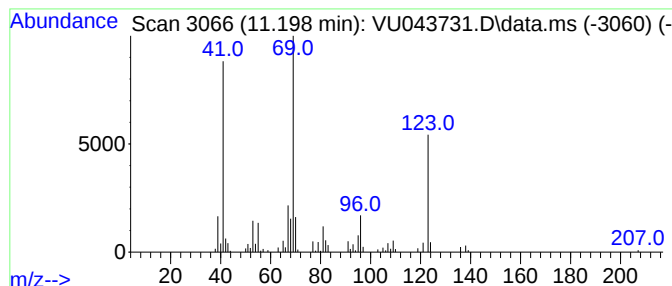
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Quant Title : VOC Analysis

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

Peak Number 15 unknown-05 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.198	4.02 ug/L	94806	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, bromo-	148	C5H9Br	000137-43-9	43
2			6-Methyl-1,5-heptadiene	110	C8H14	007270-50-0	43
3			2,6-Octadiene, 2,7-dimethyl-	138	C10H18	016736-42-8	43
4			cis-2,6-Dimethyl-2,6-octadiene	138	C10H18	002492-22-0	43
5			trans-Farnesol	222	C15H26O	000106-28-5	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043731.D
Acq On : 14 May 2021 04:15
Operator : SY/MD
Sample : M2350-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG6L5

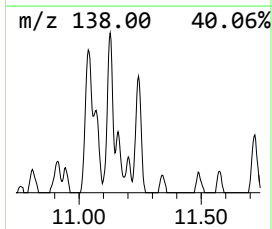
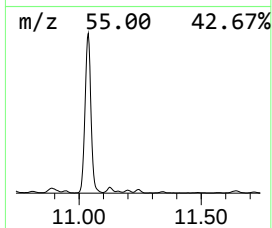
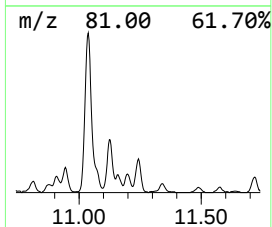
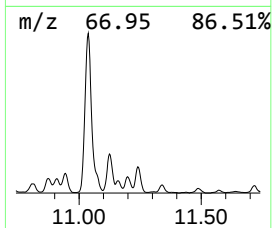
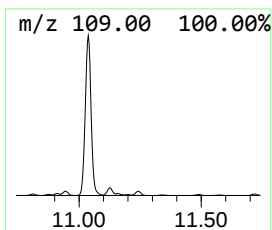
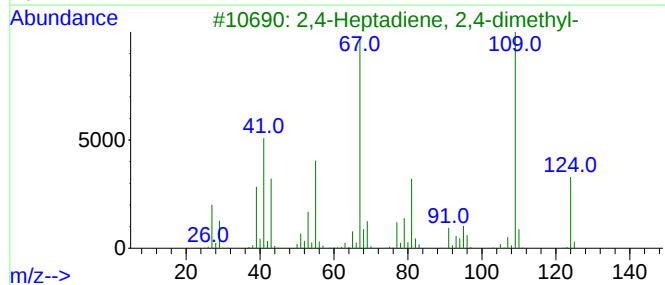
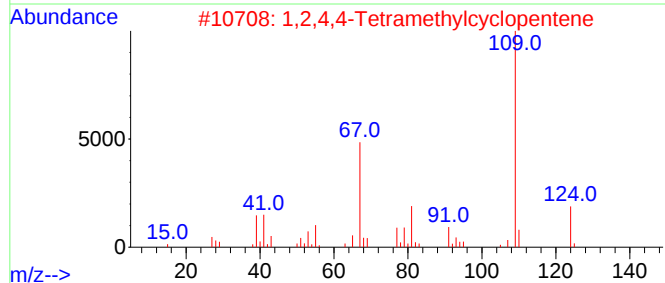
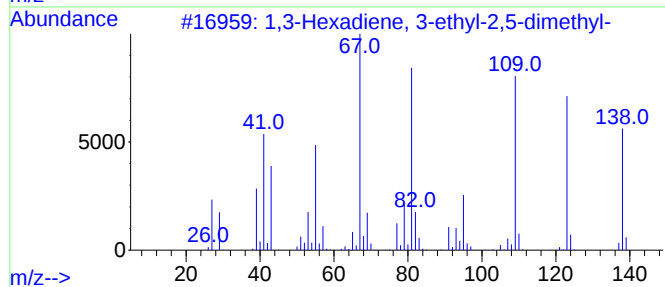
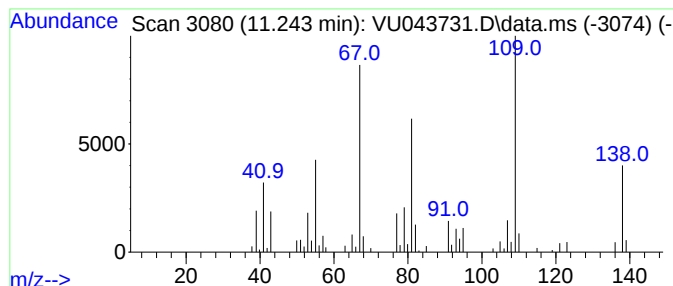
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Quant Title : VOC Analysis

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

Peak Number 16 1,3-Hexadiene, 3-ethyl-2,5-... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.243	3.37 ug/L	79369	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Hexadiene, 3-ethyl-2,5-dimet...	138	C10H18	062338-07-2	70		
2	1,2,4,4-Tetramethylcyclopentene	124	C9H16	065378-76-9	58		
3	2,4-Heptadiene, 2,4-dimethyl-	124	C9H16	074421-05-9	53		
4	1,3-Hexadiene, 2,3,5-trimethyl-	124	C9H16	061142-34-5	53		
5	3,3,5,5-Tetramethylcyclopentene	124	C9H16	038667-10-6	50		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043731.D
Acq On : 14 May 2021 04:15
Operator : SY/MD
Sample : M2350-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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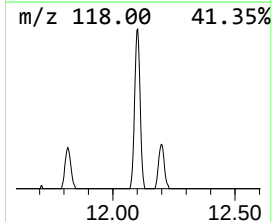
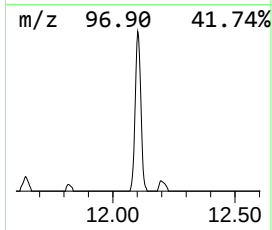
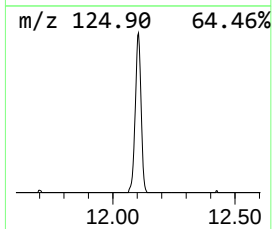
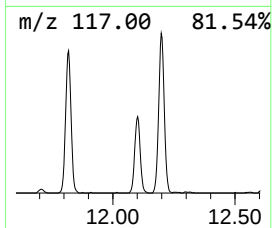
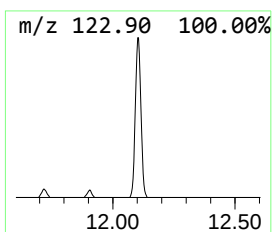
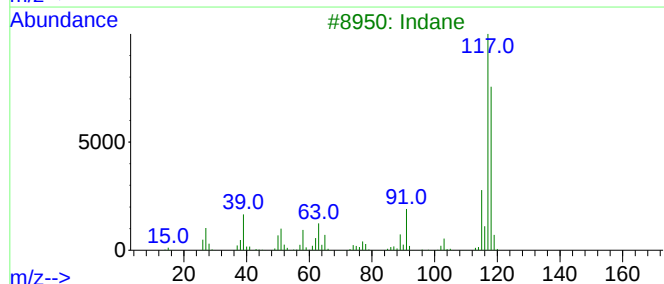
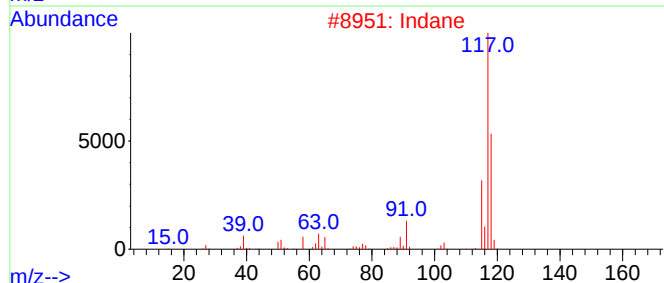
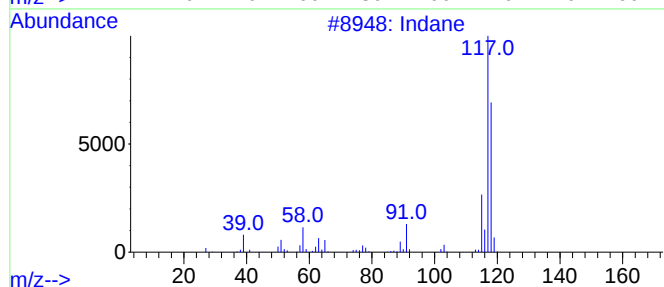
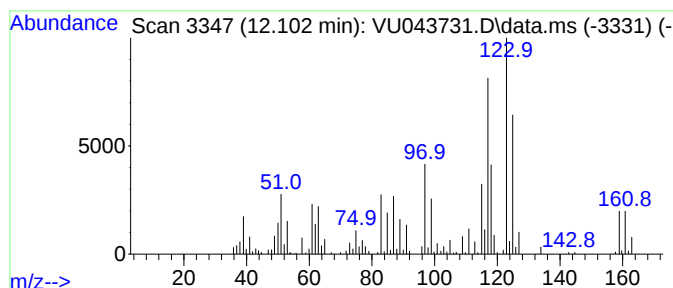
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Quant Title : VOC Analysis

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

Peak Number 17 unknown-06 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.102	9.77 ug/L	230118	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	35
2			Indane	118	C9H10	000496-11-7	20
3			Indane	118	C9H10	000496-11-7	18
4			Benzonitrile, 3-methyl-	117	C8H7N	000620-22-4	18
5			Indane	118	C9H10	000496-11-7	18



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043731.D
Acq On : 14 May 2021 04:15
Operator : SY/MD
Sample : M2350-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG6L5

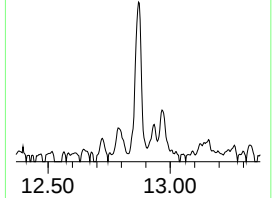
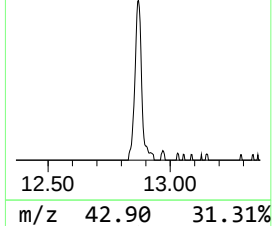
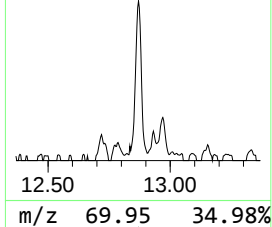
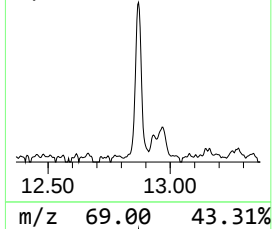
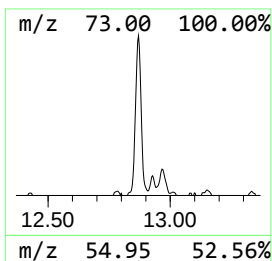
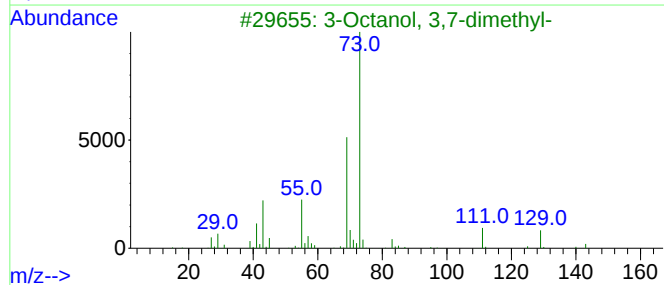
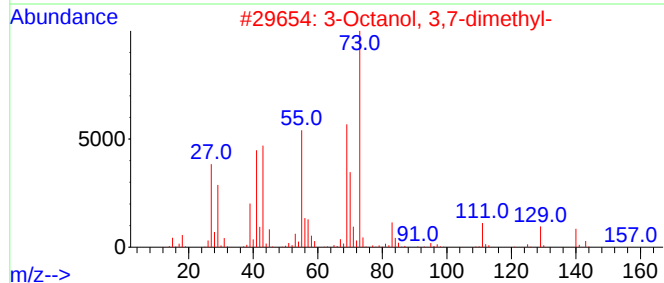
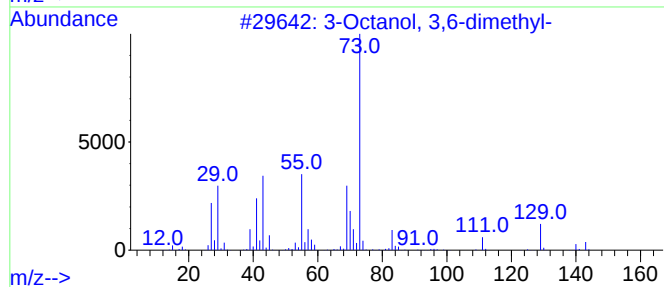
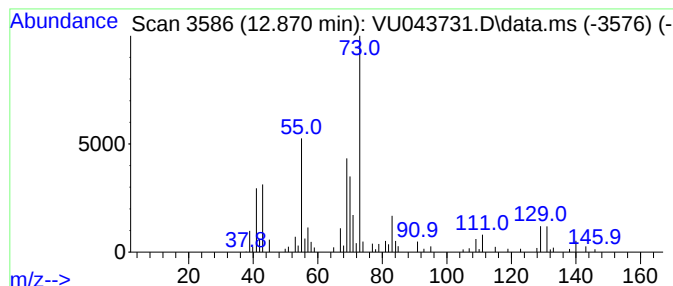
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Quant Title : VOC Analysis

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

Peak Number 18 unknown-07 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.870	2.66 ug/L	62704	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Octanol, 3,6-dimethyl-	158	C10H22O	000151-19-9	42
2			3-Octanol, 3,7-dimethyl-	158	C10H22O	000078-69-3	40
3			3-Octanol, 3,7-dimethyl-	158	C10H22O	000078-69-3	38
4			3-Octanol, 3,7-dimethyl-	158	C10H22O	000078-69-3	38
5			3-Dodecanol, 3,7,11-trimethyl-	228	C15H32O	007278-65-1	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
Data File : VU043731.D
Acq On : 14 May 2021 04:15
Operator : SY/MD
Sample : M2350-02
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 43 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BG6L5

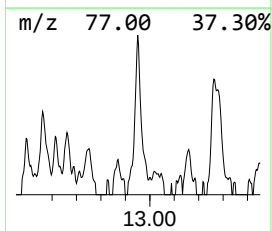
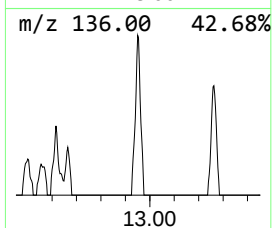
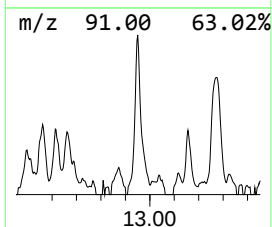
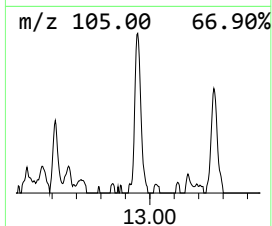
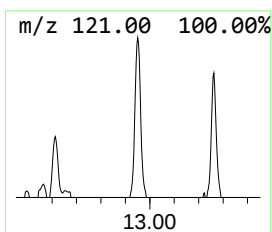
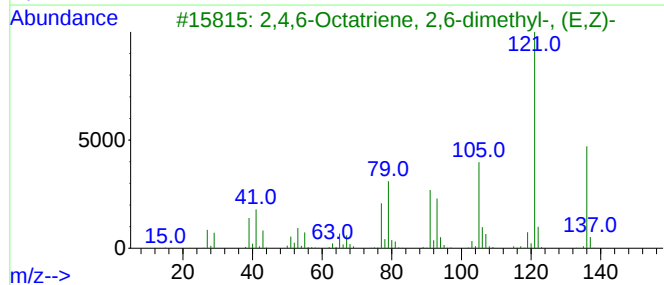
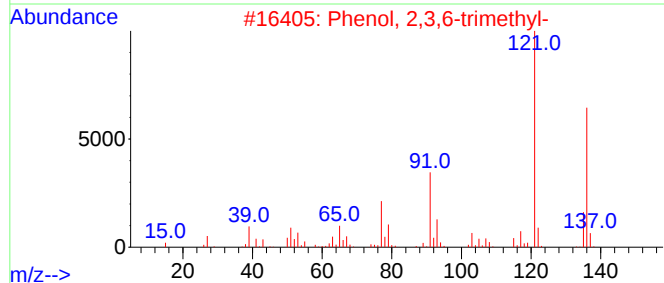
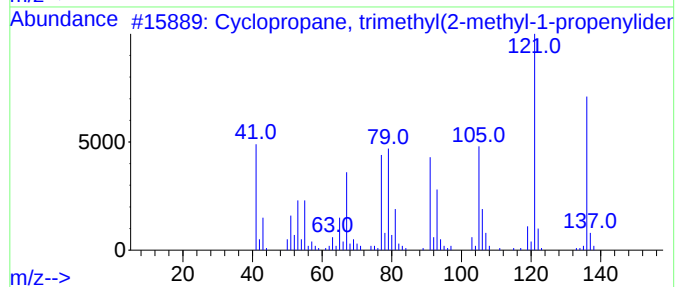
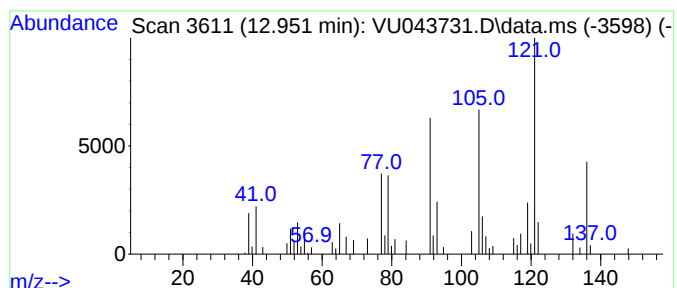
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.M
Quant Title : VOC Analysis

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

Peak Number 19 Cyclopropane, trimethyl(2-m... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.951	2.50 ug/L	58990	1,4-Dichlorobenzene-d4	11.819

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopropane, trimethyl(2-methyl...	136	C10H16	014803-30-6	87
2		Phenol, 2,3,6-trimethyl-	136	C9H12O	002416-94-6	81
3		2,4,6-Octatriene, 2,6-dimethyl-,...	136	C10H16	007216-56-0	76
4		Phenol, 2,4,6-trimethyl-	136	C9H12O	000527-60-6	76
5		1,3-Cyclopentadiene, 1,2,3,4,5-p...	136	C10H16	004045-44-7	76



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051421\
 Data File : VU043731.D
 Acq On : 14 May 2021 04:15
 Operator : SY/MD
 Sample : M2350-02
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BG6L5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051421WMA.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
Isopropyl Alcohol	2.764	3.2	ug/L	61426	1	6.256	958615	50.0
2-Propanol, 2-m...	3.182	8.9	ug/L	171555	1	6.256	958615	50.0
Diisopropyl ether	4.002	8.9	ug/L	171239	1	6.256	958615	50.0
2(1H)-Pyrimidin...	6.922	31.6	ug/L	605140	1	6.256	958615	50.0
(DEL) Alkane: S...	7.346	21.7	ug/L	416424	1	6.256	958615	50.0
(DEL) Alkane: S...	7.523	29.0	ug/L	555409	1	6.256	958615	50.0
Furan, tetrahyd...	7.719	27.0	ug/L	517750	1	6.256	958615	50.0
2-Hexanol, 2,5-...	10.262	154.4	ug/L	4116860	2	9.423	1333500	50.0
unknown-01	10.549	4.6	ug/L	122348	2	9.423	1333500	50.0
unknown-02	10.896	6.2	ug/L	146434	3	11.819	1177980	50.0
unknown-03	10.944	3.3	ug/L	76684	3	11.819	1177980	50.0
unknown-04	11.037	223.9	ug/L	5274690	3	11.819	1177980	50.0
1,3-Heptadiene,...	11.124	6.2	ug/L	145407	3	11.819	1177980	50.0
unknown-05	11.198	4.0	ug/L	94806	3	11.819	1177980	50.0
1,3-Hexadiene, ...	11.243	3.4	ug/L	79369	3	11.819	1177980	50.0
unknown-06	12.102	9.8	ug/L	230118	3	11.819	1177980	50.0
unknown-07	12.870	2.7	ug/L	62704	3	11.819	1177980	50.0
Cyclopropane, t...	12.951	2.5	ug/L	58990	3	11.819	1177980	50.0