

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050721\
 Data File : VV021329.D
 Acq On : 07 May 2021 16:36
 Operator : SY/MD
 Sample : M2320-01DL 20X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 F3A00DL

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\SFAMVLM050321WMA.M

Title : VOC Analysis

Signal : TIC: VV021329.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	77	83	101	rVB	302283	317224	12.90%	1.402%
2	1.568	158	164	175	rVB	243662	274862	11.18%	1.214%
3	1.635	178	185	199	rVB	131597	162437	6.61%	0.718%
4	2.108	323	332	359	rVB	605654	924882	37.62%	4.087%
5	2.500	442	454	462	rBV4	45559	92686	3.77%	0.410%
6	2.770	523	538	570	rVB	1001906	2124666	86.43%	9.388%
7	2.918	581	584	587	rVB5	1984	1326	0.05%	0.006%
8	2.941	587	591	597	rVB6	2232	1821	0.07%	0.008%
9	3.082	631	635	637	rVB3	1115	843	0.03%	0.004%
10	3.121	645	647	652	rVV5	1022	773	0.03%	0.003%
11	3.243	681	685	687	rBV2	718	544	0.02%	0.002%
12	3.330	710	712	716	rBV4	1197	883	0.04%	0.004%
13	3.375	724	726	732	rVB3	1673	927	0.04%	0.004%
14	3.429	739	743	745	rVB3	1217	608	0.02%	0.003%
15	3.494	758	763	765	rBV3	1778	1338	0.05%	0.006%
16	3.532	765	775	777	rBV8	3007	3854	0.16%	0.017%
17	3.593	791	794	798	rVB5	1706	1100	0.04%	0.005%
18	3.632	802	806	807	rBV3	1153	817	0.03%	0.004%
19	3.744	837	841	843	rBV5	2292	1919	0.08%	0.008%
20	3.905	879	891	917	rBV2	126412	442737	18.01%	1.956%
21	4.265	1000	1003	1004	rBV2	1390	709	0.03%	0.003%
22	4.352	1014	1030	1057	rBV	459154	1155531	47.00%	5.106%
23	4.584	1100	1102	1104	rBV3	1125	495	0.02%	0.002%
24	4.603	1104	1108	1109	rBV3	1589	1011	0.04%	0.004%
25	4.764	1148	1158	1179	rVB6	47212	120107	4.89%	0.531%
26	5.050	1230	1247	1268	rBV2	947955	2458322	100.00%	10.862%
27	5.481	1378	1381	1385	rBV4	1867	1480	0.06%	0.007%
28	5.619	1410	1424	1455	rBV	831415	1673016	68.06%	7.392%
29	5.915	1503	1516	1532	rBV7	58380	150422	6.12%	0.665%
30	6.072	1550	1565	1596	rBV2	527124	1092582	44.44%	4.828%
31	6.400	1664	1667	1668	rBV2	1362	673	0.03%	0.003%
32	6.458	1681	1685	1688	rBV4	4391	3184	0.13%	0.014%
33	6.526	1701	1706	1707	rBV5	1486	1351	0.05%	0.006%
34	6.783	1771	1786	1796	rBV8	19956	43878	1.78%	0.194%
35	6.989	1840	1850	1866	rBV3	328443	597010	24.29%	2.638%
36	7.320	1942	1953	1972	rBV	1169089	2028742	82.53%	8.964%

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050321WMA.M

Title : VOC Analysis

37	7.625	2039	2048	2069	rBV	234521	418169	17.01%	1.848%
38	7.985	2151	2160	2173	rVB10	11872	23521	0.96%	0.104%
39	8.095	2184	2194	2223	rBV2	515230	1043489	42.45%	4.611%
40	8.577	2341	2344	2347	rBV5	1446	1015	0.04%	0.004%
41	8.789	2408	2410	2411	rBV3	1237	545	0.02%	0.002%
42	8.857	2419	2431	2458	rBV	1239424	2039174	82.95%	9.010%
43	9.107	2506	2509	2511	rBV4	2800	1927	0.08%	0.009%
44	9.152	2514	2523	2533	rVB4	5202	10460	0.43%	0.046%
45	9.416	2602	2605	2607	rBV	1132	789	0.03%	0.003%
46	9.439	2609	2612	2613	rBV2	954	475	0.02%	0.002%
47	9.657	2676	2680	2682	rVV4	864	598	0.02%	0.003%
48	9.754	2706	2710	2717	rBV9	2916	3011	0.12%	0.013%
49	9.783	2717	2719	2723	rBV4	1853	1271	0.05%	0.006%
50	9.860	2740	2743	2745	rBV3	1876	1252	0.05%	0.006%
51	9.943	2762	2769	2772	rBV6	3052	3416	0.14%	0.015%
52	9.982	2779	2781	2784	rVB4	1501	691	0.03%	0.003%
53	10.056	2800	2804	2805	rBV4	752	616	0.03%	0.003%
54	10.069	2805	2808	2809	rBV	1730	868	0.04%	0.004%
55	10.095	2814	2816	2819	rVB4	1281	569	0.02%	0.003%
56	10.114	2819	2822	2823	rBV2	2852	1690	0.07%	0.007%
57	10.220	2844	2855	2874	rBV	722874	1160278	47.20%	5.127%
58	10.297	2877	2879	2882	rBV4	1706	1053	0.04%	0.005%
59	10.455	2924	2928	2930	rBV5	1106	841	0.03%	0.004%
60	10.551	2954	2958	2964	rVV6	3584	4468	0.18%	0.020%
61	10.796	3032	3034	3036	rBV3	1024	457	0.02%	0.002%
62	10.924	3069	3074	3083	rVB7	8349	12664	0.52%	0.056%
63	11.127	3133	3137	3140	rBV5	1528	1479	0.06%	0.007%
64	11.194	3153	3158	3165	rBV9	4080	5808	0.24%	0.026%
65	11.255	3166	3177	3198	rBV	1289779	2014249	81.94%	8.900%
66	11.513	3254	3257	3260	rBV5	1392	904	0.04%	0.004%
67	11.532	3260	3263	3264	rBV2	970	561	0.02%	0.002%
68	11.632	3282	3294	3319	rBV	1309356	2095906	85.26%	9.261%
69	11.911	3378	3381	3384	rBV3	1306	638	0.03%	0.003%
70	12.008	3405	3411	3417	rBV7	2079	2743	0.11%	0.012%
71	12.140	3450	3452	3454	rBV3	903	514	0.02%	0.002%
72	12.165	3457	3460	3462	rBV4	1382	785	0.03%	0.003%
73	12.239	3481	3483	3485	rBV3	977	580	0.02%	0.003%
74	12.281	3493	3496	3499	rBV4	2346	1482	0.06%	0.007%
75	12.307	3500	3504	3509	rVB7	4155	3668	0.15%	0.016%
76	12.339	3512	3514	3518	rVB2	2071	1161	0.05%	0.005%

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77	12.361	3518	3521	3522	rBV	1176	758	0.03%	0.003%
78	12.419	3537	3539	3542	rBV2	1096	668	0.03%	0.003%
79	12.442	3542	3546	3549	rVB6	2238	1738	0.07%	0.008%
80	12.551	3574	3580	3588	rBV6	2043	2224	0.09%	0.010%
81	12.606	3594	3597	3600	rBV4	1245	1098	0.04%	0.005%
82	12.657	3604	3613	3620	rBV9	9721	16257	0.66%	0.072%
83	12.747	3638	3641	3643	rBV3	951	711	0.03%	0.003%
84	12.995	3716	3718	3720	rBV3	1666	919	0.04%	0.004%
85	13.037	3728	3731	3734	rBV5	1618	1313	0.05%	0.006%
86	13.072	3740	3742	3745	rVB2	1243	617	0.03%	0.003%
87	13.139	3760	3763	3767	rBV4	1169	953	0.04%	0.004%
88	13.275	3798	3805	3806	rBV6	7652	8732	0.36%	0.039%
89	13.374	3834	3836	3839	rVB4	1367	733	0.03%	0.003%
90	13.410	3844	3847	3851	rVB6	2076	1182	0.05%	0.005%
91	13.519	3874	3881	3890	rBV4	13388	17816	0.72%	0.079%
92	13.625	3911	3914	3916	rBV2	1760	1036	0.04%	0.005%
93	13.693	3932	3935	3937	rBV2	861	666	0.03%	0.003%
94	13.754	3946	3954	3965	rVB9	10134	17561	0.71%	0.078%
95	13.895	3997	3998	4002	rBV3	1235	761	0.03%	0.003%
96	13.985	4023	4026	4029	rVB5	2141	1302	0.05%	0.006%
97	14.117	4064	4067	4070	rBV5	1571	944	0.04%	0.004%
98	14.239	4101	4105	4106	rBV4	1933	1225	0.05%	0.005%
99	14.956	4324	4328	4332	rBV6	2567	2778	0.11%	0.012%
100	15.432	4473	4476	4479	rBV3	2441	1644	0.07%	0.007%

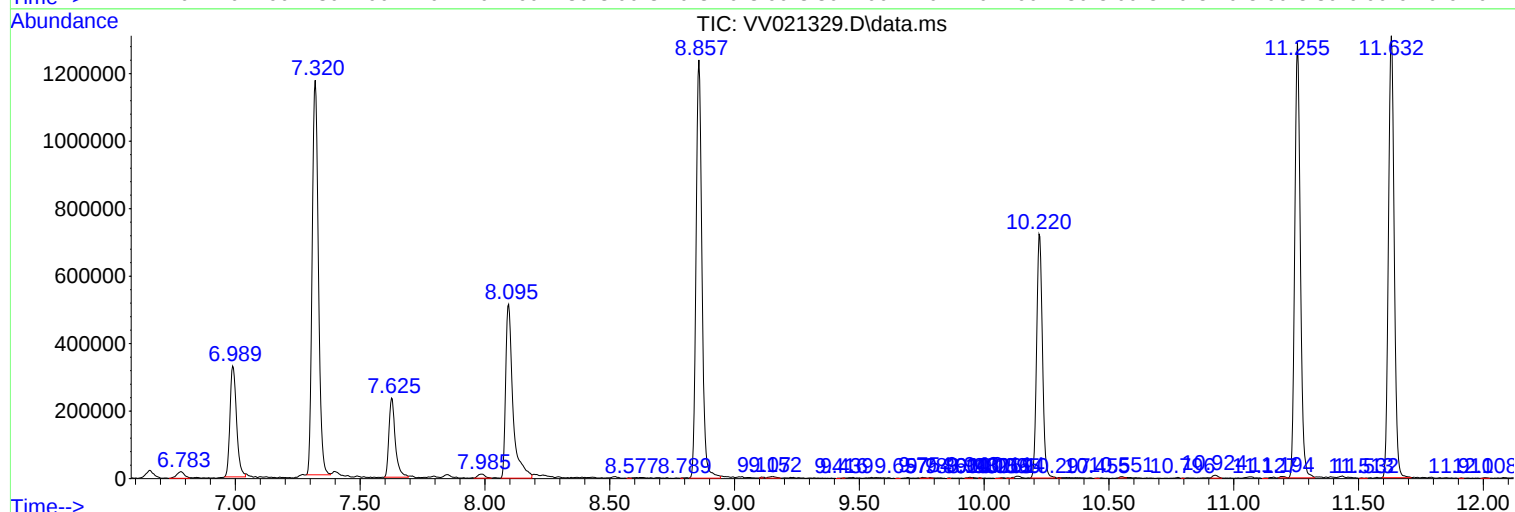
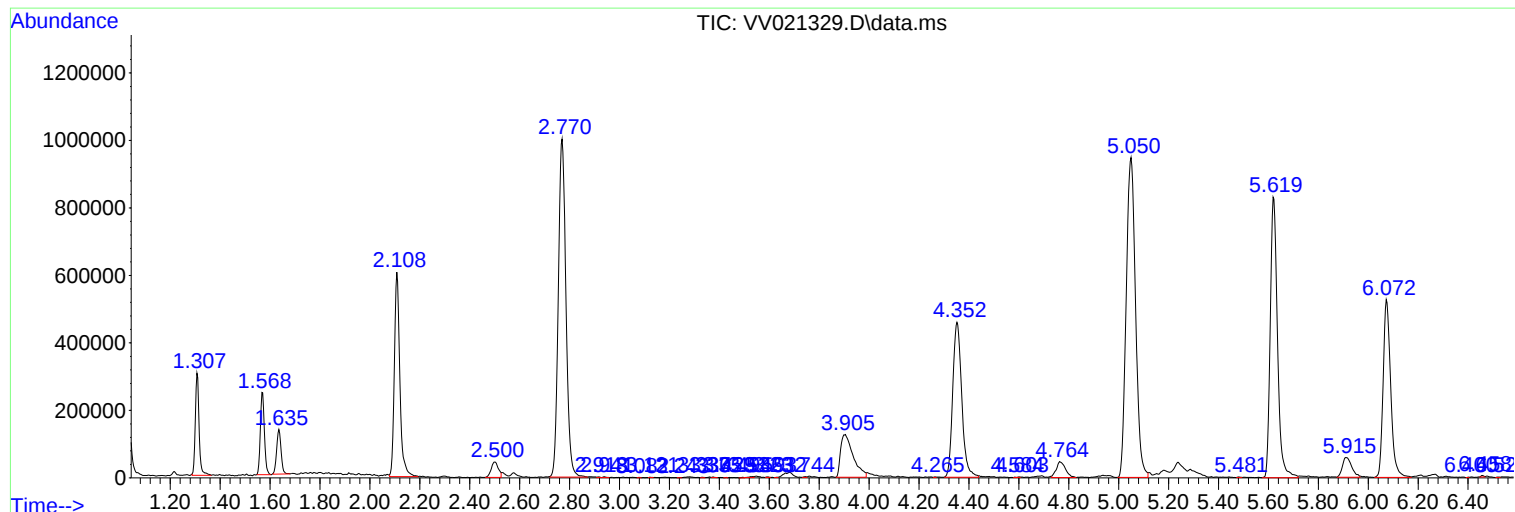
Sum of corrected areas: 22632181

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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050321WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050721\
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Instrument :
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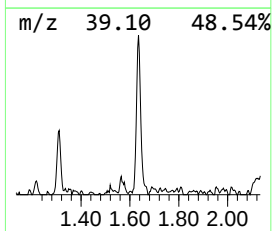
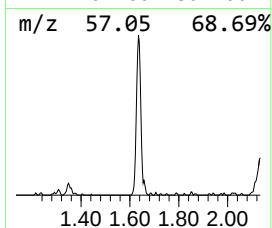
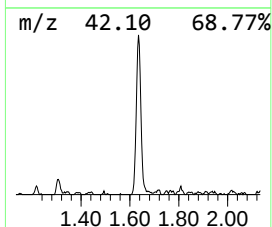
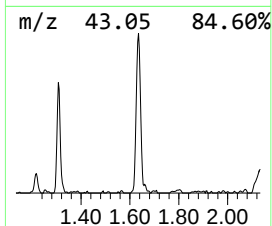
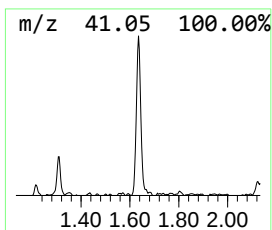
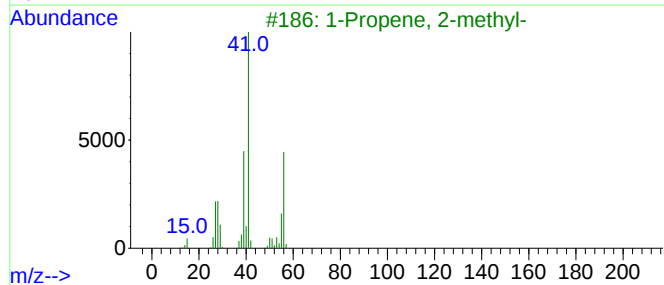
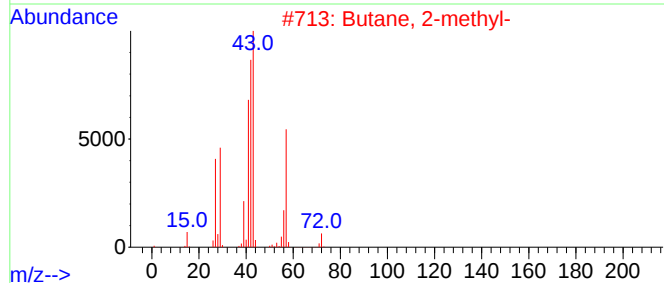
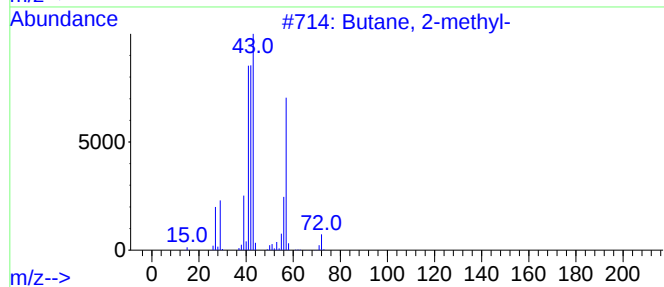
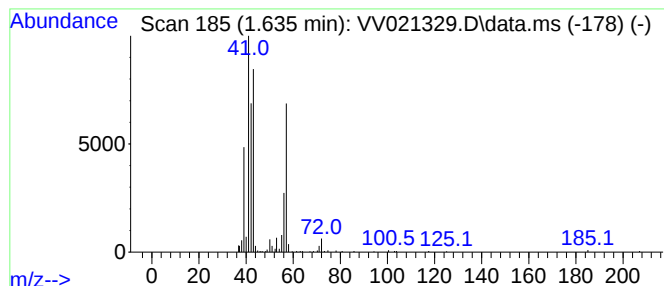
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.635	4.85 ug/L	162437	1,4-Difluorobenzene	5.622

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	70
2			Butane, 2-methyl-	72	C5H12	000078-78-4	49
3			1-Propene, 2-methyl-	56	C4H8	000115-11-7	46
4			Butane, 2-methyl-	72	C5H12	000078-78-4	43
5			2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	38



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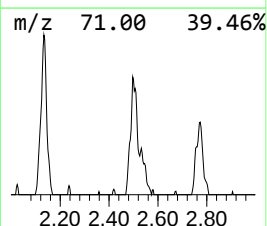
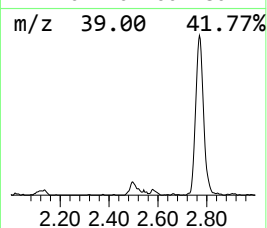
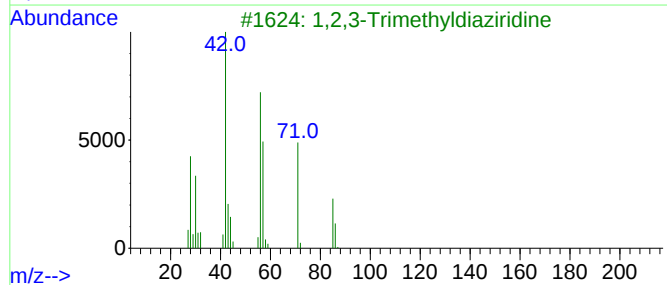
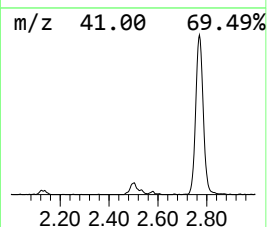
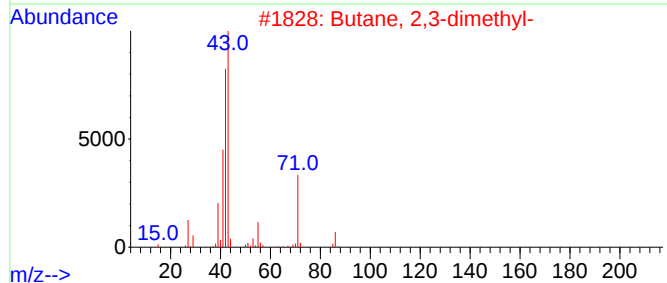
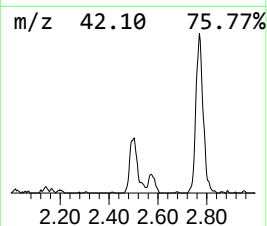
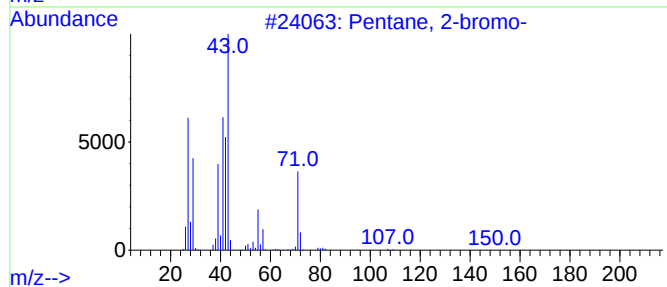
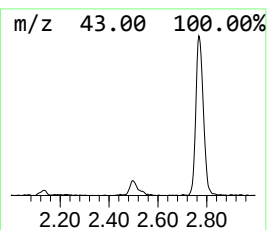
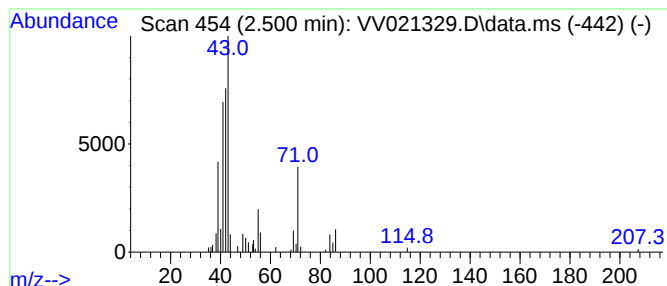
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentane, 2-bromo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.500	2.77 ug/L	92686	1,4-Difluorobenzene	5.622

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2-bromo-	150	C5H11Br	000107-81-3	59
2			Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	52
3			1,2,3-Trimethyldiaziridine	86	C4H10N2	113604-56-1	47
4			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	47
5			Methylamine, N-(1-propylbutylide...	127	C8H17N	010599-78-7	39



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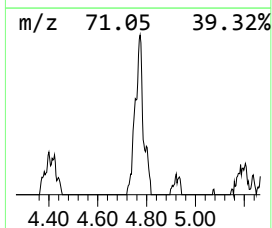
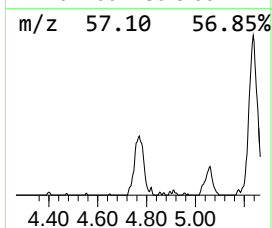
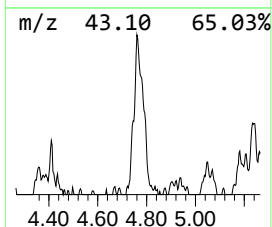
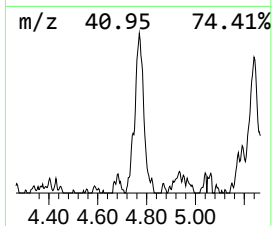
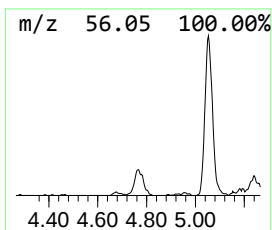
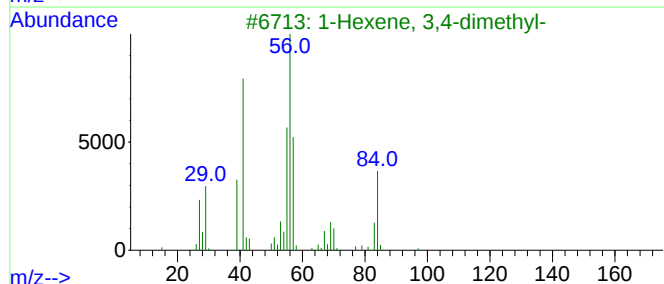
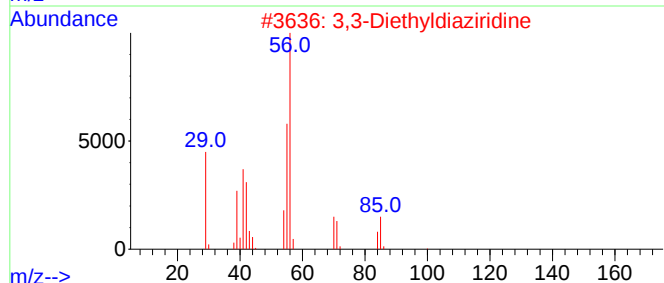
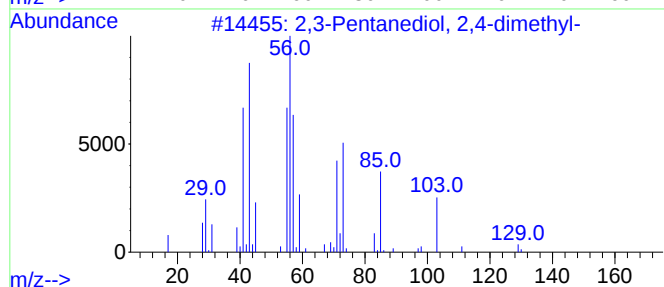
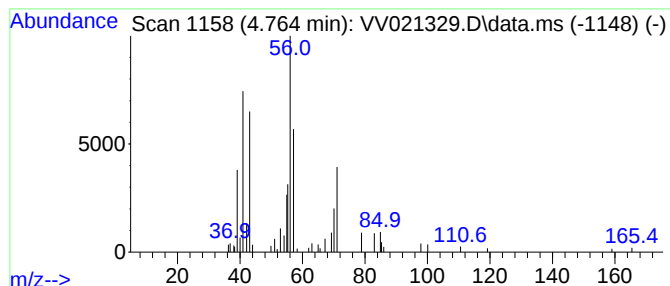
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Quant Title : VOC Analysis

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

Peak Number 3 2,3-Pentenediol, 2,4-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.764	3.59 ug/L	120107	1,4-Difluorobenzene	5.622

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Pentenediol, 2,4-dimethyl-	132	C7H16O2	066225-53-4	59		
2	3,3-Diethyldiaziridine	100	C5H12N2	052175-94-7	50		
3	1-Hexene, 3,4-dimethyl-	112	C8H16	016745-94-1	43		
4	1-Hexene, 3,4-dimethyl-	112	C8H16	016745-94-1	43		
5	2-Hexene, 5-methyl-, (E)-	98	C7H14	007385-82-2	43		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050721\
Data File : VV021329.D
Acq On : 07 May 2021 16:36
Operator : SY/MD
Sample : M2320-01DL 20X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F3A00DL

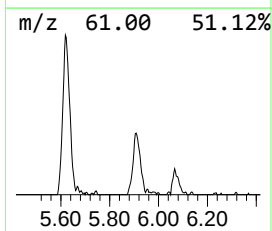
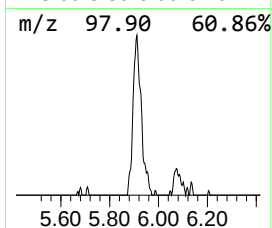
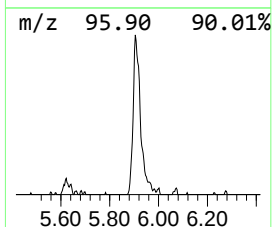
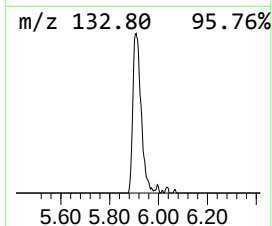
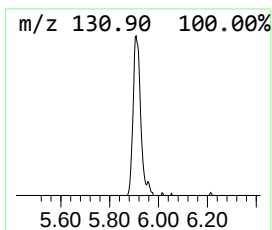
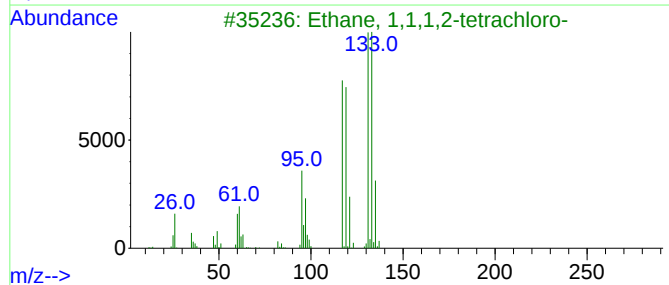
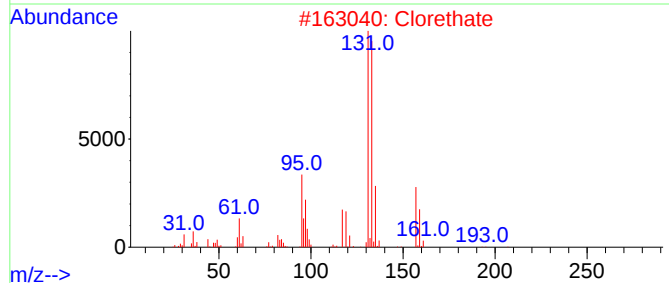
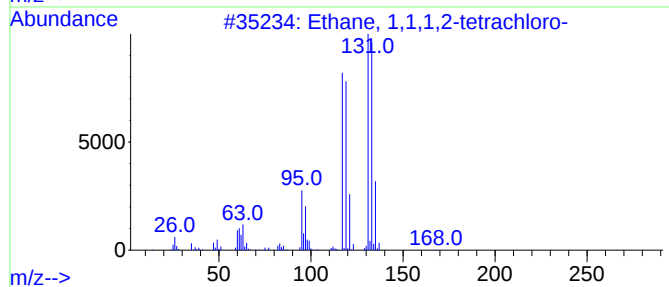
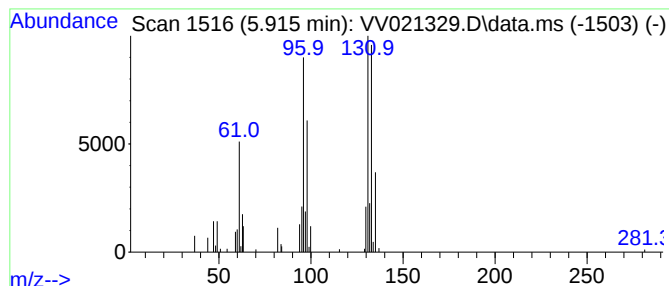
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050321WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.915	4.50 ug/L	150422	1,4-Difluorobenzene	5.622

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	38
2			Clorethate	322	C5H4Cl6O3	005634-37-7	33
3			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	32
4			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	32
5			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV050721\
Data File : VV021329.D
Acq On : 07 May 2021 16:36
Operator : SY/MD
Sample : M2320-01DL 20X
Misc : 5.0mL/MSVOA_V/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
F3A00DL

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM050321WMA.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
(DEL) Alkane: S...	1.635	4.8	ug/L	162437	1	5.622	1673020	50.0
Pentane, 2-bromo-	2.500	2.8	ug/L	92686	1	5.622	1673020	50.0
2,3-Pentanediol...	4.764	3.6	ug/L	120107	1	5.622	1673020	50.0
unknown-01	5.915	4.5	ug/L	150422	1	5.622	1673020	50.0