

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051022\
 Data File : VV025872.D
 Acq On : 10 May 2022 19:55
 Operator : SY/MD
 Sample : N2714-05ME
 Misc : 5.49g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 EW2X6ME

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\SFAMVLM051022WMA.M
 Title : VOC Analysis

Signal : TIC: VV025872.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.738	522	528	532	rVB7	789	910	0.78%	0.178%
2	2.761	532	535	538	rBV3	472	396	0.34%	0.078%
3	3.034	615	620	621	rBV2	436	303	0.26%	0.059%
4	3.066	627	630	632	rBV	253	161	0.14%	0.032%
5	3.089	635	637	640	rVB	443	216	0.18%	0.042%
6	3.105	640	642	648	rBV2	325	223	0.19%	0.044%
7	3.143	652	654	656	rBV	245	149	0.13%	0.029%
8	3.172	660	663	666	rBV	229	197	0.17%	0.039%
9	3.188	666	668	669	rBV	401	206	0.18%	0.040%
10	3.275	693	695	697	rVV2	366	177	0.15%	0.035%
11	3.298	697	702	705	rVB3	332	356	0.30%	0.070%
12	3.330	707	712	713	rBV3	304	255	0.22%	0.050%
13	3.552	777	781	782	rBV2	387	192	0.16%	0.038%
14	3.693	819	825	829	rBV2	348	319	0.27%	0.062%
15	3.719	829	833	836	rVB2	274	206	0.18%	0.040%
16	3.751	840	843	846	rBV3	216	164	0.14%	0.032%
17	3.822	862	865	868	rBV3	350	207	0.18%	0.041%
18	3.863	875	878	884	rVB	321	249	0.21%	0.049%
19	3.982	896	915	916	rBV5	3672	7009	5.97%	1.373%
20	4.539	1086	1088	1089	rBV	527	200	0.17%	0.039%
21	4.667	1125	1128	1131	rVB	452	218	0.19%	0.043%
22	4.760	1155	1157	1161	rVB2	248	165	0.14%	0.032%
23	4.851	1183	1185	1188	rBV3	277	162	0.14%	0.032%
24	4.873	1188	1192	1194	rBV3	303	215	0.18%	0.042%
25	4.928	1206	1209	1212	rVB2	409	256	0.22%	0.050%
26	4.992	1224	1229	1231	rBV	287	230	0.20%	0.045%
27	5.047	1231	1246	1268	rBV3	46319	117374	100.00%	22.986%
28	5.172	1282	1285	1288	rBV2	605	518	0.44%	0.101%
29	5.252	1307	1310	1311	rBV	406	211	0.18%	0.041%
30	5.297	1322	1324	1327	rVB3	474	256	0.22%	0.050%
31	5.342	1327	1338	1343	rBV6	4605	8614	7.34%	1.687%
32	5.625	1418	1426	1445	rBV	7462	16464	14.03%	3.224%
33	5.863	1497	1500	1504	rBV2	318	200	0.17%	0.039%
34	5.915	1507	1516	1518	rBV7	2064	2518	2.15%	0.493%
35	5.973	1532	1534	1537	rBV3	477	297	0.25%	0.058%
36	5.992	1537	1540	1541	rBV4	1320	790	0.67%	0.155%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051022WMA.M
 Title : VOC Analysis

37	6.072	1558	1565	1587	rVB2	22188	47005	40.05%	9.205%
38	6.304	1632	1637	1640	rVB4	341	305	0.26%	0.060%
39	6.320	1640	1642	1645	rBV2	284	158	0.13%	0.031%
40	6.423	1672	1674	1676	rVB	463	188	0.16%	0.037%
41	6.474	1687	1690	1694	rVB	355	283	0.24%	0.055%
42	6.519	1701	1704	1705	rBV	322	167	0.14%	0.033%
43	6.561	1714	1717	1718	rBV	278	146	0.12%	0.029%
44	6.593	1724	1727	1731	rVB2	422	256	0.22%	0.050%
45	6.793	1787	1789	1791	rBV	586	298	0.25%	0.058%
46	6.828	1798	1800	1804	rVB2	388	181	0.15%	0.035%
47	6.850	1804	1807	1810	rBV	283	165	0.14%	0.032%
48	6.899	1820	1822	1828	rVB2	305	242	0.21%	0.047%
49	6.928	1828	1831	1834	rBV	458	269	0.23%	0.053%
50	6.944	1834	1836	1841	rVB4	386	318	0.27%	0.062%
51	6.998	1841	1853	1874	rBV4	9297	21965	18.71%	4.302%
52	7.166	1901	1905	1907	rBV2	225	182	0.16%	0.036%
53	7.246	1919	1930	1936	rBV4	530	849	0.72%	0.166%
54	7.320	1943	1953	1975	rBV	37783	73752	62.84%	14.443%
55	7.564	2028	2029	2032	rVB	403	171	0.15%	0.033%
56	7.587	2032	2036	2038	rVB	319	204	0.17%	0.040%
57	7.638	2043	2052	2070	rBV4	6097	14540	12.39%	2.847%
58	7.796	2093	2101	2102	rBV3	802	728	0.62%	0.143%
59	7.918	2135	2139	2140	rBV	264	197	0.17%	0.039%
60	7.985	2155	2160	2161	rBV	240	174	0.15%	0.034%
61	8.056	2176	2182	2184	rBV2	219	244	0.21%	0.048%
62	8.130	2194	2205	2235	rBV3	8760	27880	23.75%	5.460%
63	8.400	2287	2289	2291	rVB	476	191	0.16%	0.037%
64	8.426	2296	2297	2299	rBV	421	170	0.14%	0.033%
65	8.471	2309	2311	2313	rBV	287	145	0.12%	0.028%
66	8.516	2323	2325	2329	rBV2	293	144	0.12%	0.028%
67	8.558	2335	2338	2341	rBV2	254	155	0.13%	0.030%
68	8.661	2368	2370	2373	rVB2	419	199	0.17%	0.039%
69	8.683	2373	2377	2379	rBV2	229	171	0.15%	0.033%
70	8.760	2398	2401	2404	rBV	283	174	0.15%	0.034%
71	8.863	2423	2433	2450	rBV3	11643	24406	20.79%	4.780%
72	8.992	2468	2473	2475	rBV2	264	188	0.16%	0.037%
73	9.001	2475	2476	2479	rVB2	418	187	0.16%	0.037%
74	9.149	2520	2522	2526	rVB	288	151	0.13%	0.030%
75	9.175	2526	2530	2532	rBV2	313	166	0.14%	0.033%
76	9.323	2572	2576	2580	rBV3	252	267	0.23%	0.052%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051022WMA.M
 Title : VOC Analysis

77	9.410	2600	2603	2605	rBV2	241	146	0.12%	0.029%
78	9.535	2641	2642	2647	rVB2	251	148	0.13%	0.029%
79	9.593	2657	2660	2664	rVB2	315	184	0.16%	0.036%
80	9.635	2670	2673	2675	rBV2	269	178	0.15%	0.035%
81	9.940	2765	2768	2771	rVB2	345	241	0.21%	0.047%
82	10.120	2820	2824	2827	rBV	342	220	0.19%	0.043%
83	10.223	2844	2856	2869	rBV2	25399	44282	37.73%	8.672%
84	10.294	2876	2878	2883	rBV4	422	256	0.22%	0.050%
85	10.532	2947	2952	2955	rBV2	415	275	0.23%	0.054%
86	10.548	2955	2957	2960	rBV2	301	166	0.14%	0.033%
87	10.574	2960	2965	2966	rBV3	2690	1945	1.66%	0.381%
88	10.834	3044	3046	3050	rBV2	200	146	0.12%	0.029%
89	10.892	3062	3064	3068	rVB	340	185	0.16%	0.036%
90	11.259	3169	3178	3190	rBV2	13269	22035	18.77%	4.315%
91	11.339	3200	3203	3205	rVB	448	201	0.17%	0.039%
92	11.365	3209	3211	3218	rVB2	261	199	0.17%	0.039%
93	11.628	3283	3293	3307	rBV	36892	59866	51.00%	11.724%
94	11.776	3336	3339	3343	rBV3	476	279	0.24%	0.055%
95	12.197	3466	3470	3471	rBV	259	191	0.16%	0.037%
96	12.371	3522	3524	3528	rVB2	373	175	0.15%	0.034%
97	12.561	3581	3583	3586	rBV	406	339	0.29%	0.066%
98	12.654	3610	3612	3616	rBV	472	255	0.22%	0.050%
99	13.210	3783	3785	3788	rBV	333	174	0.15%	0.034%
100	13.702	3934	3938	3942	rVB3	455	376	0.32%	0.074%

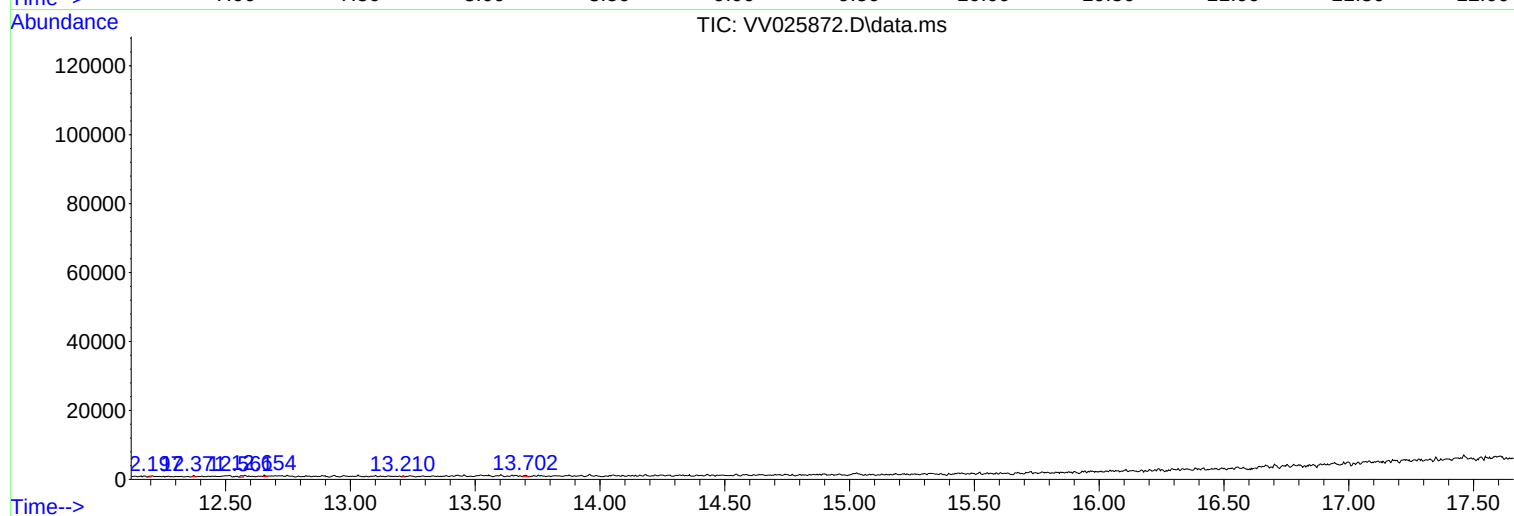
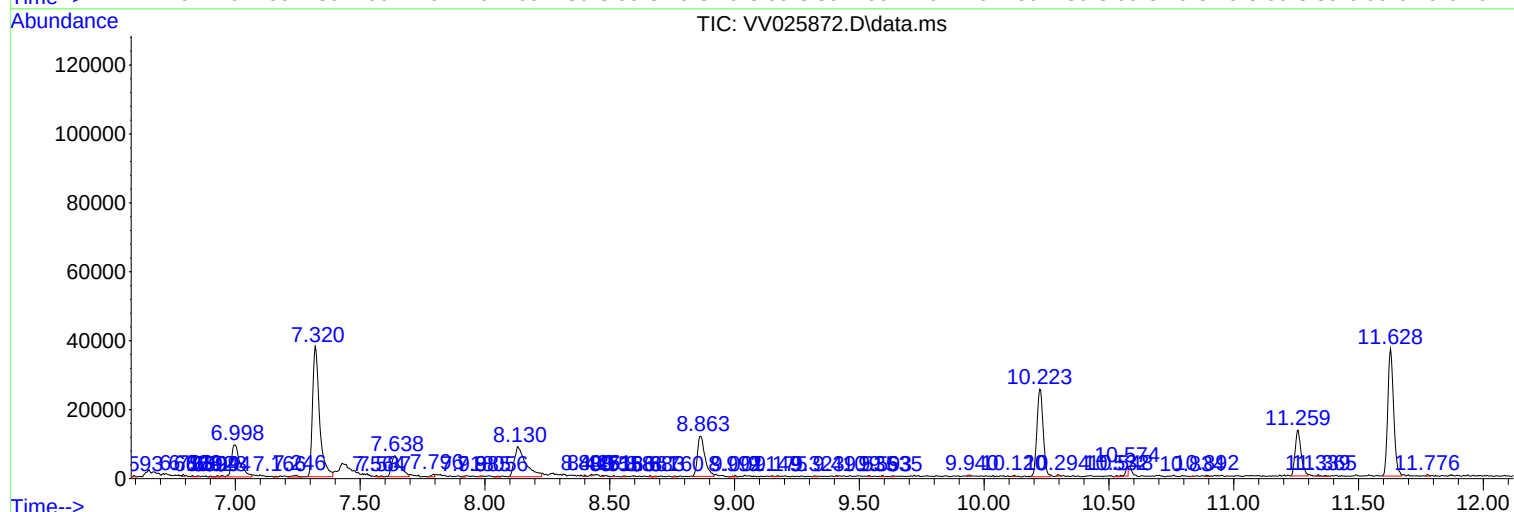
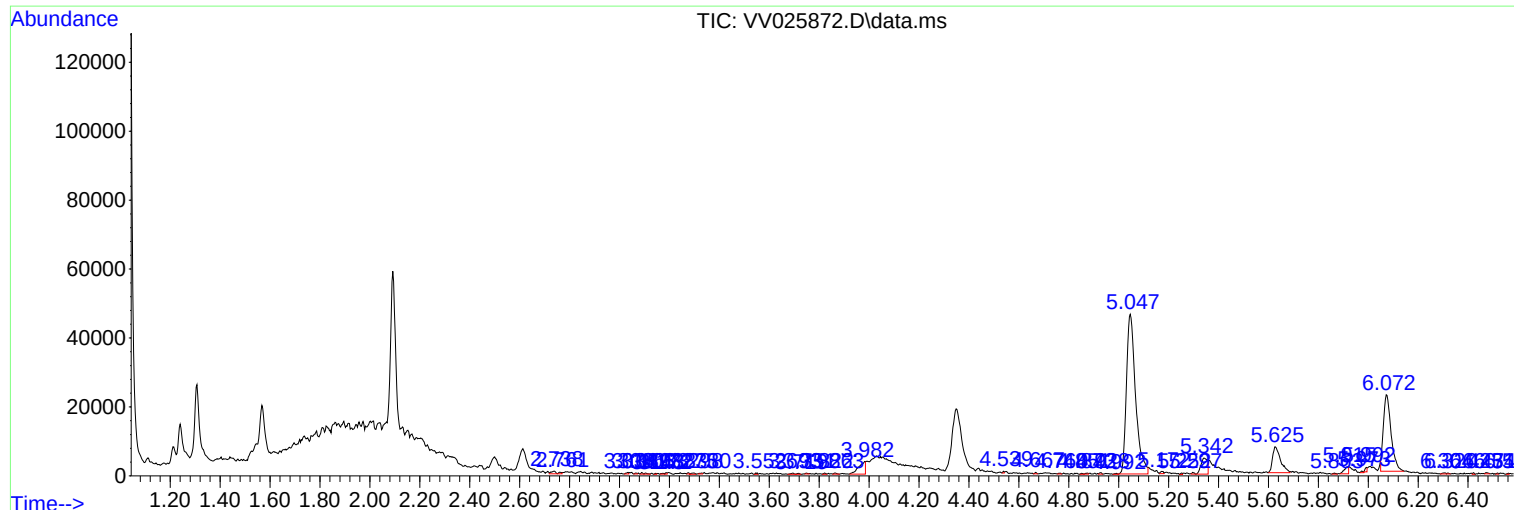
Sum of corrected areas: 510626

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Instrument :
MSVOA_V
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051022WMA.M
Quant Title : VOC Analysis

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



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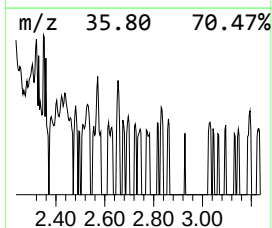
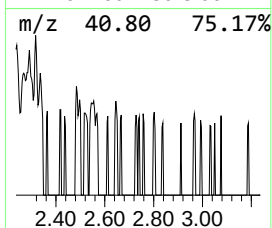
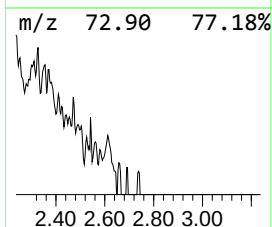
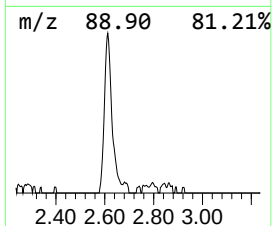
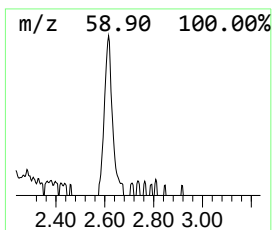
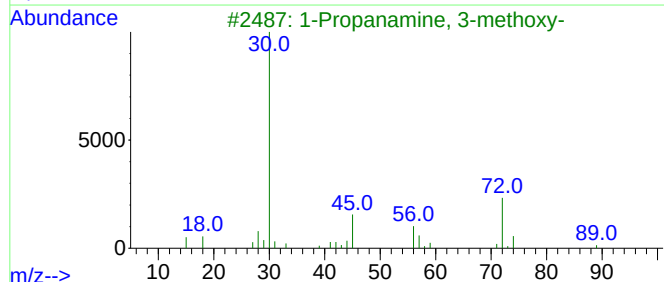
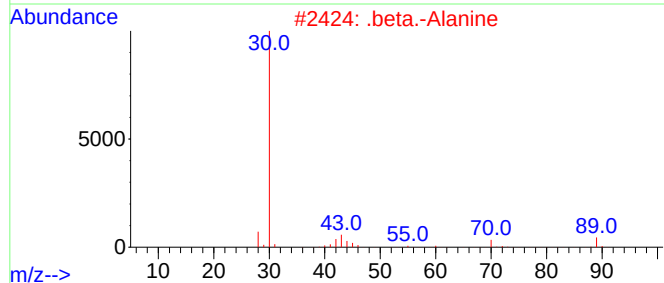
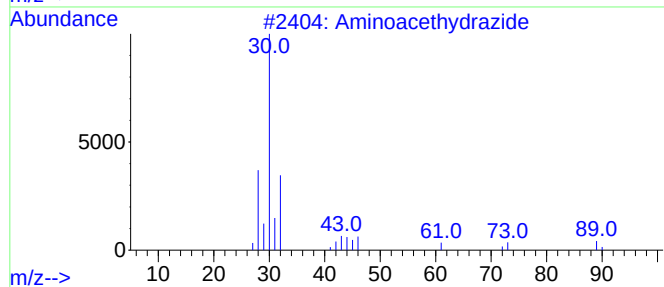
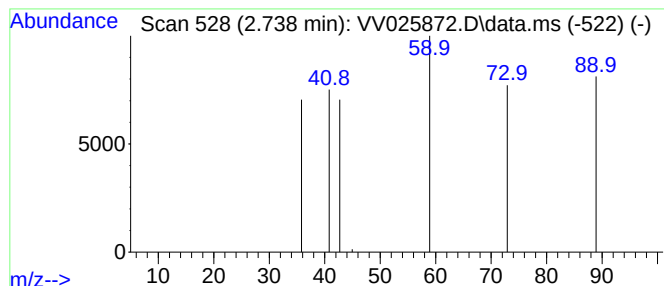
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051022WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.738	2.76 ug/L	910	1,4-Difluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Aminoacethydrazide	89	C2H7N3O	014379-80-7	3
2			.beta.-Alanine	89	C3H7NO2	000107-95-9	3
3			1-Propanamine, 3-methoxy-	89	C4H11NO	005332-73-0	3
4			Ethane, 1-ethoxy-1-methoxy-	104	C5H12O2	010471-14-4	2
5			L-Threonine, O-methyl-, methyl e...	147	C6H13NO3	1000452-62-7	2



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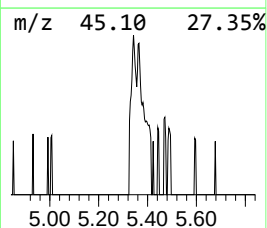
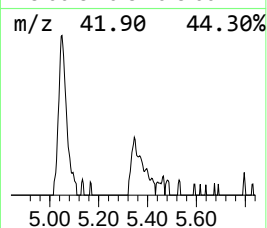
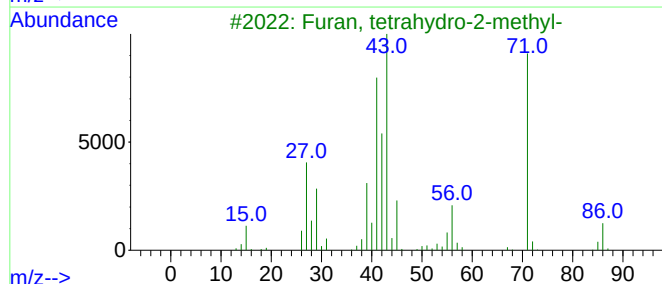
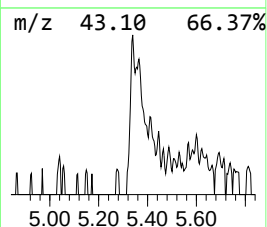
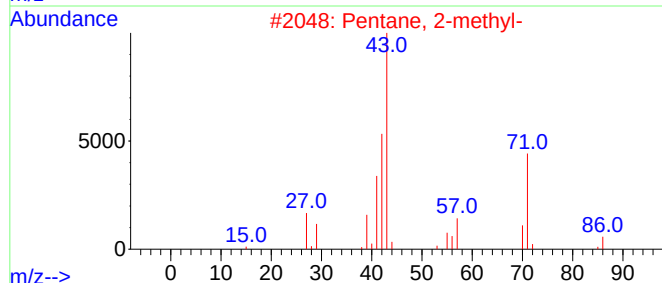
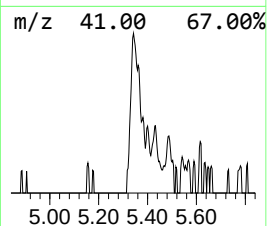
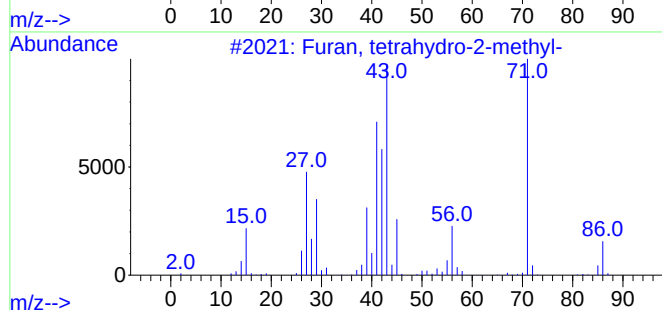
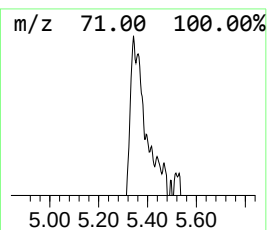
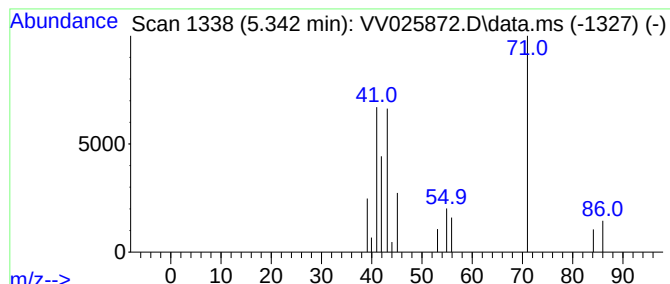
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051022WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.342	26.16 ug/L	8614	1,4-Difluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	72
2			Pentane, 2-methyl-	86	C6H14	000107-83-5	64
3			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	58
4			1-Propene, 1-methoxy-2-methyl-	86	C5H10O	017574-84-4	50
5			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	47



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ClientSampleId :
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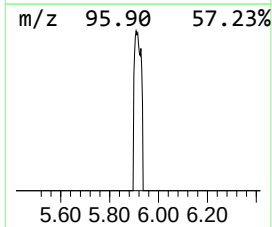
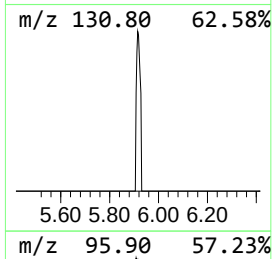
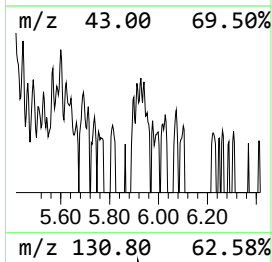
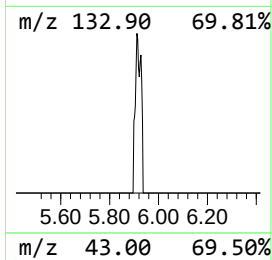
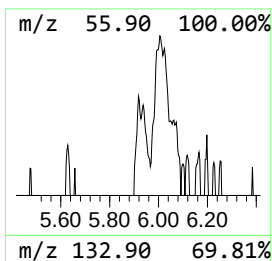
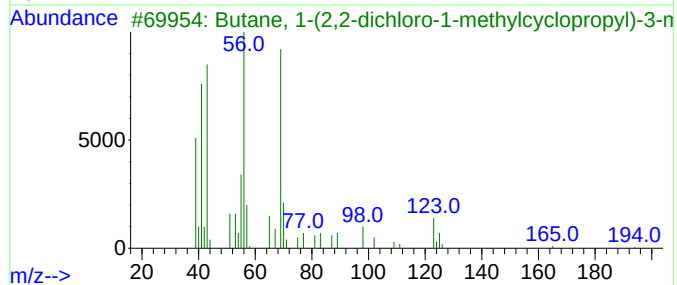
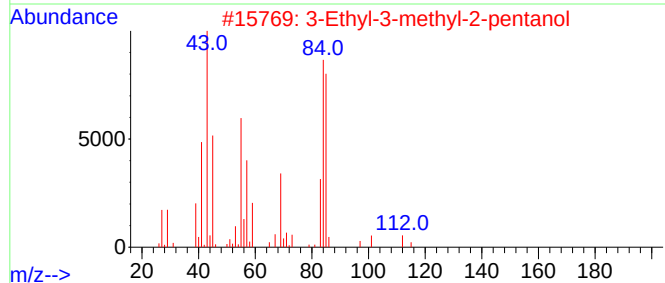
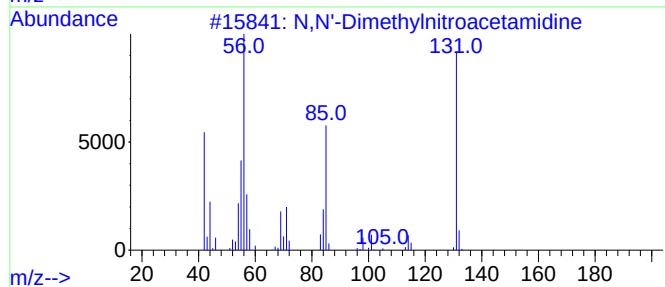
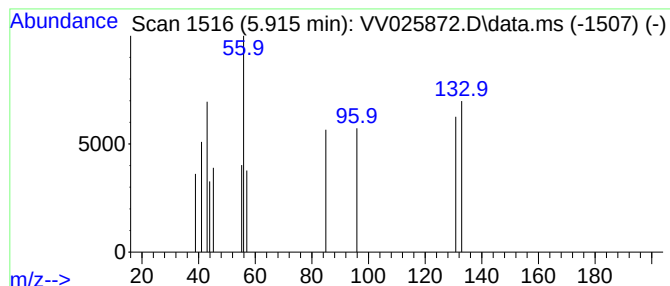
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051022WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.915	7.65 ug/L	2518	1,4-Difluorobenzene	5.629

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N,N'-Dimethylnitroacetamide	131	C4H9N3O2	054252-45-8	37
2			3-Ethyl-3-methyl-2-pentanol	130	C8H18O	066576-22-5	10
3			Butane, 1-(2,2-dichloro-1-methyl...	194	C9H16Cl2	024551-81-3	9
4			Heptane, 2,3-epoxy-	114	C7H14O	014925-96-3	9
5			Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV051022\
Data File : VV025872.D
Acq On : 10 May 2022 19:55
Operator : SY/MD
Sample : N2714-05ME
Misc : 5.49g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EW2X6ME

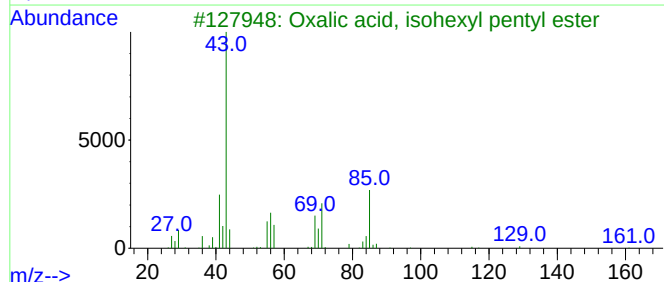
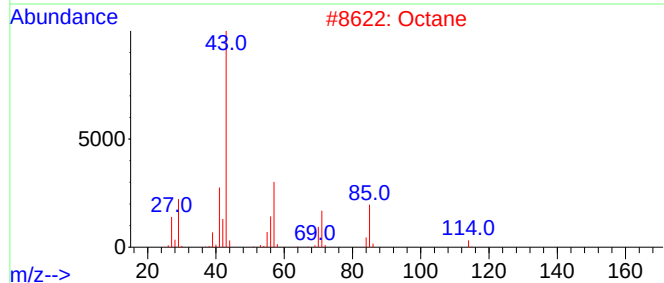
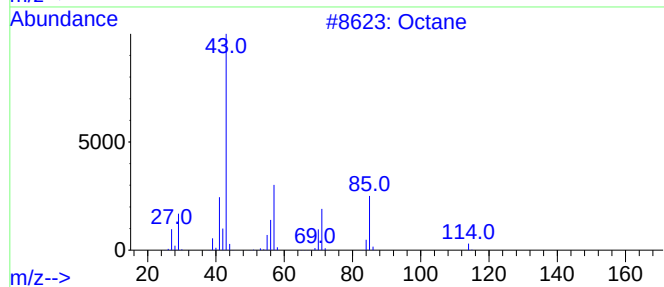
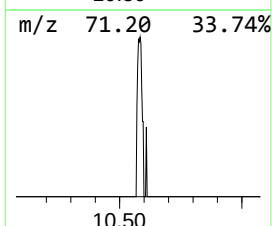
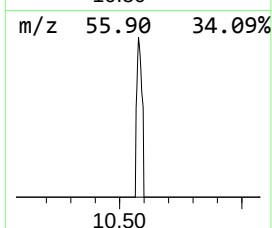
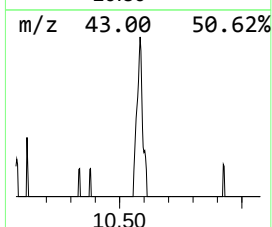
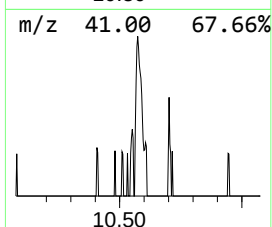
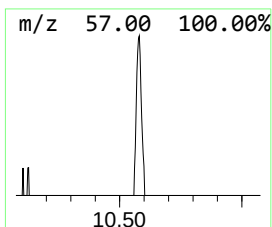
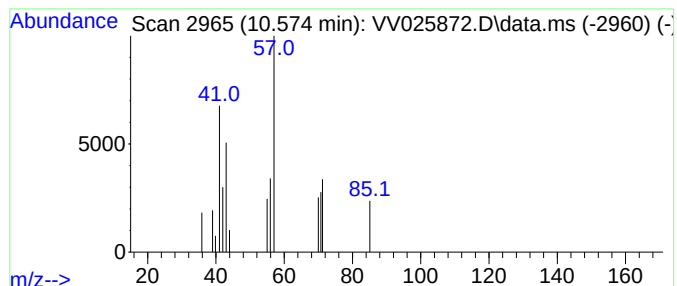
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Quant Title : VOC Analysis

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.574	4.41 ug/L	1945	1,4-Dichlorobenzene-d4	11.259

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane			114	C8H18	000111-65-9	50
2	Octane			114	C8H18	000111-65-9	39
3	Oxalic acid, isohexyl pentyl ester			244	C13H24O4	1000309-32-8	36
4	Heptane, 2,4-dimethyl-			128	C9H20	002213-23-2	36
5	Hexane, 2,3,5-trimethyl-			128	C9H20	001069-53-0	36



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW051022\
Data File : VW025872.D
Acq On : 10 May 2022 19:55
Operator : SY/MD
Sample : N2714-05ME
Misc : 5.49g/5.0mL/100uL/5.00mL/MSVOA_V/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
EW2X6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM051022WMA.M
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
unknown-01	2.738	2.8	ug/L	910	1	5.629	16464	50.0
Furan, tetrahyd...	5.342	26.2	ug/L	8614	1	5.629	16464	50.0
unknown-02	5.915	7.7	ug/L	2518	1	5.629	16464	50.0
(DEL) Alkane: S...	10.574	4.4	ug/L	1945	3	11.259	22035	50.0