

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102522\
 Data File : VU051491.D
 Acq On : 25 Oct 2022 17:15
 Operator : JC/MD
 Sample : N5258-07ME
 Misc : 6.48g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GBLN6ME

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\SFAMULM102022WMA.M
 Title : VOC Analysis

Signal : TIC: VU051491.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.481	38	44	50	rBV3	7164	9571	0.46%	0.048%
2	1.597	72	80	101	rVB	143086	261251	12.51%	1.318%
3	1.761	117	131	132	rBV5	21639	31999	1.53%	0.161%
4	1.845	141	157	190	rBV	629007	955328	45.74%	4.819%
5	2.131	238	246	259	rVB2	38647	55977	2.68%	0.282%
6	2.526	357	369	395	rBV	366011	618872	29.63%	3.122%
7	2.636	397	403	415	rVB3	5067	9198	0.44%	0.046%
8	2.957	493	503	515	rBV	10725	20901	1.00%	0.105%
9	3.028	515	525	548	rVB2	11870	28043	1.34%	0.141%
10	3.176	554	571	586	rBV2	44088	105674	5.06%	0.533%
11	4.636	1009	1025	1070	rBV	150600	492569	23.58%	2.485%
12	5.057	1138	1156	1184	rBV	354593	803112	38.45%	4.051%
13	5.446	1267	1277	1287	rVB4	3373	6193	0.30%	0.031%
14	5.581	1308	1319	1328	rVV8	3208	6510	0.31%	0.033%
15	5.713	1340	1360	1385	rBV2	791083	2033489	97.35%	10.258%
16	5.980	1431	1443	1452	rBV7	5313	10627	0.51%	0.054%
17	6.124	1475	1488	1499	rBV4	9585	18709	0.90%	0.094%
18	6.243	1507	1525	1553	rBV	659216	1300781	62.27%	6.562%
19	6.687	1648	1663	1692	rBV	467490	952156	45.58%	4.803%
20	6.803	1692	1699	1708	rVV7	4055	6477	0.31%	0.033%
21	6.857	1708	1716	1726	rVB8	4176	7372	0.35%	0.037%
22	7.066	1768	1781	1792	rVB5	8764	16998	0.81%	0.086%
23	7.192	1809	1820	1822	rBV4	4646	6337	0.30%	0.032%
24	7.227	1824	1831	1846	rVB6	12572	24286	1.16%	0.123%
25	7.420	1881	1891	1899	rBV6	3591	5390	0.26%	0.027%
26	7.494	1899	1914	1922	rBV3	37057	67175	3.22%	0.339%
27	7.565	1922	1936	1957	rVV	221210	426585	20.42%	2.152%
28	7.655	1960	1964	1971	rVB6	5078	6384	0.31%	0.032%
29	7.896	2015	2039	2061	rBV2	1102765	2088783	100.00%	10.537%
30	8.092	2091	2100	2104	rBV9	8230	13874	0.66%	0.070%
31	8.124	2104	2110	2118	rVB3	22435	29779	1.43%	0.150%
32	8.179	2118	2127	2139	rBV	149392	269909	12.92%	1.362%
33	8.365	2176	2185	2194	rVB10	5198	8960	0.43%	0.045%
34	8.430	2194	2205	2209	rBV10	2960	4590	0.22%	0.023%
35	8.472	2213	2218	2227	rVB6	2903	4700	0.23%	0.024%
36	8.536	2227	2238	2253	rBV10	10831	24692	1.18%	0.125%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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\SFAMULM102022WMA.M
 Title : VOC Analysis

37	8.645	2255	2272	2300	rBV	605649	1240945	59.41%	6.260%
38	8.799	2317	2320	2333	rVB7	7962	9648	0.46%	0.049%
39	8.861	2336	2339	2346	rVB2	6567	7606	0.36%	0.038%
40	8.922	2346	2358	2387	rVB	116468	234002	11.20%	1.180%
41	9.070	2392	2404	2412	rBV4	25586	45357	2.17%	0.229%
42	9.118	2413	2419	2425	rVB4	7672	8831	0.42%	0.045%
43	9.163	2425	2433	2440	rBV6	12152	20185	0.97%	0.102%
44	9.211	2442	2448	2458	rVB2	15341	24780	1.19%	0.125%
45	9.333	2468	2486	2498	rBV4	30320	58192	2.79%	0.294%
46	9.420	2498	2513	2527	rBV	943426	1666669	79.79%	8.408%
47	9.558	2547	2556	2573	rVB	8548	23248	1.11%	0.117%
48	9.664	2573	2589	2595	rBV	10891	28978	1.39%	0.146%
49	9.709	2596	2603	2606	rVV8	12477	20160	0.97%	0.102%
50	9.745	2607	2614	2635	rVB4	39446	82280	3.94%	0.415%
51	9.873	2642	2654	2665	rBV5	13784	27140	1.30%	0.137%
52	10.028	2687	2702	2713	rBV5	13803	34792	1.67%	0.176%
53	10.131	2721	2734	2735	rBV8	4762	8945	0.43%	0.045%
54	10.250	2760	2771	2783	rBV4	53780	104472	5.00%	0.527%
55	10.356	2798	2804	2810	rBV7	7898	11943	0.57%	0.060%
56	10.465	2831	2838	2849	rVB7	4059	8897	0.43%	0.045%
57	10.529	2851	2858	2862	rBV6	6494	9541	0.46%	0.048%
58	10.626	2875	2888	2893	rBV8	17583	32811	1.57%	0.166%
59	10.693	2903	2909	2917	rBV7	4231	6207	0.30%	0.031%
60	10.758	2917	2929	2939	rBV	792521	1273472	60.97%	6.424%
61	10.809	2939	2945	2959	rVB4	66462	112401	5.38%	0.567%
62	10.877	2961	2966	2972	rBV7	3812	4488	0.21%	0.023%
63	10.951	2982	2989	2993	rBV7	5695	5976	0.29%	0.030%
64	11.024	3001	3012	3020	rBV8	26576	52439	2.51%	0.265%
65	11.114	3030	3040	3054	rVB2	39960	72522	3.47%	0.366%
66	11.185	3054	3062	3073	rVB5	9720	15608	0.75%	0.079%
67	11.246	3073	3081	3089	rBV5	6849	10887	0.52%	0.055%
68	11.304	3091	3099	3112	rVB5	9571	20444	0.98%	0.103%
69	11.414	3124	3133	3142	rBV2	60945	93815	4.49%	0.473%
70	11.642	3197	3204	3215	rVB10	12879	22427	1.07%	0.113%
71	11.716	3216	3227	3233	rBV10	9565	18533	0.89%	0.093%
72	11.812	3245	3257	3271	rBV	975548	1563115	74.83%	7.885%
73	11.986	3304	3311	3323	rBV9	17925	32361	1.55%	0.163%
74	12.092	3331	3344	3351	rBV9	6869	17168	0.82%	0.087%
75	12.195	3363	3376	3391	rBV	918823	1507992	72.19%	7.607%
76	12.327	3409	3417	3426	rBV2	43862	62794	3.01%	0.317%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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Min Area: 0 % of largest Peak

Start Thrs: 0.2

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM102022WMA.M
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77	12.381	3428	3434	3447	rVB2	14493	30710	1.47%	0.155%
78	12.471	3456	3462	3463	rBV6	3612	4039	0.19%	0.020%
79	12.664	3515	3522	3526	rBV7	9370	13317	0.64%	0.067%
80	12.767	3548	3554	3564	rVB10	7090	10676	0.51%	0.054%
81	12.944	3598	3609	3624	rVB10	10253	27455	1.31%	0.138%
82	13.040	3630	3639	3653	rVB10	9353	21385	1.02%	0.108%
83	13.114	3655	3662	3664	rBV7	5879	7105	0.34%	0.036%
84	13.430	3752	3760	3781	rVB6	35565	84449	4.04%	0.426%
85	13.584	3800	3808	3818	rBV2	37024	59113	2.83%	0.298%
86	13.735	3845	3855	3861	rBV10	4140	7953	0.38%	0.040%
87	13.838	3879	3887	3896	rBV10	7580	15235	0.73%	0.077%
88	13.896	3903	3905	3916	rVB9	3063	3847	0.18%	0.019%
89	13.995	3933	3936	3944	rVB8	8007	8705	0.42%	0.044%
90	14.092	3961	3966	3969	rBV2	7799	9425	0.45%	0.048%
91	14.188	3988	3996	4010	rVB3	22205	37751	1.81%	0.190%
92	14.449	4070	4077	4085	rBV3	16351	22638	1.08%	0.114%
93	14.571	4108	4115	4124	rVB3	5154	7592	0.36%	0.038%
94	15.217	4306	4316	4326	rBV7	13362	31917	1.53%	0.161%
95	15.343	4349	4355	4361	rBV3	4169	6367	0.30%	0.032%
96	15.407	4370	4375	4387	rVB5	14748	24561	1.18%	0.124%
97	15.548	4413	4419	4428	rVB4	12472	18748	0.90%	0.095%
98	16.185	4614	4617	4623	rVB9	3837	3966	0.19%	0.020%
99	16.413	4680	4688	4693	rVB8	5882	9780	0.47%	0.049%
100	17.069	4887	4892	4906	rVB4	13177	21220	1.02%	0.107%

Sum of corrected areas: 19823276

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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBLN6ME

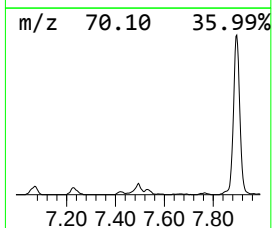
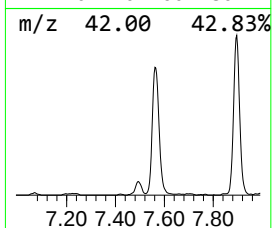
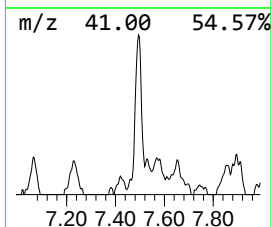
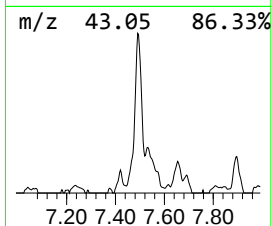
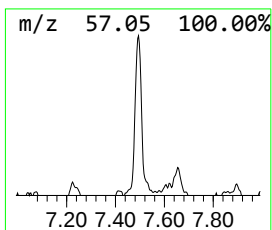
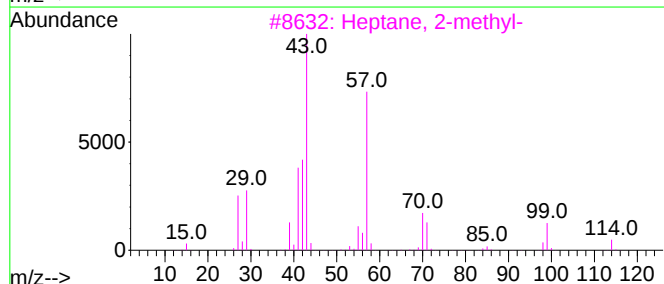
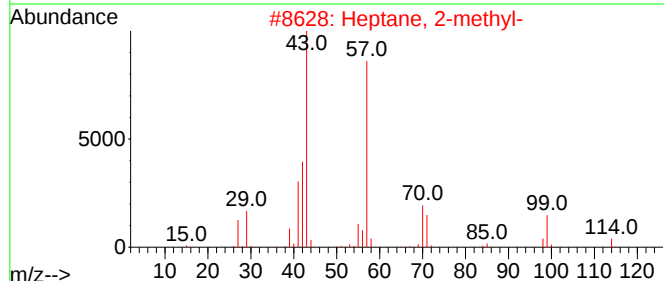
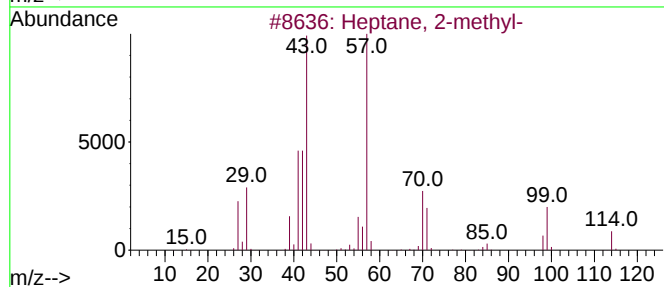
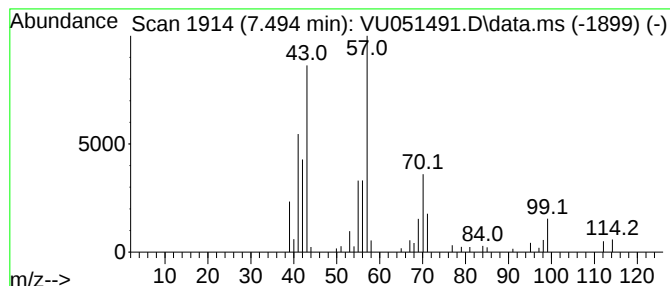
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM102022WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.494	2.58 ug/L	67175	1,4-Difluorobenzene	6.243

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2-methyl-	114	C8H18	000592-27-8	68
2			Heptane, 2-methyl-	114	C8H18	000592-27-8	68
3			Heptane, 2-methyl-	114	C8H18	000592-27-8	64
4			Hexane, 2,5-dimethyl-	114	C8H18	000592-13-2	58
5			Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	50



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Misc : 6.48g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBLN6ME

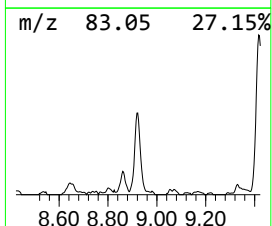
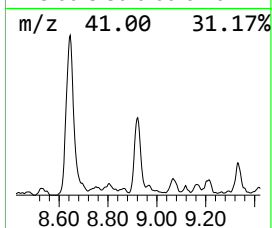
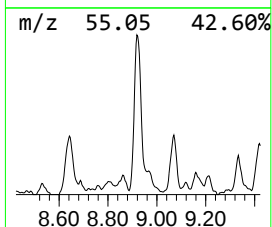
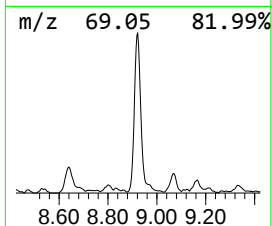
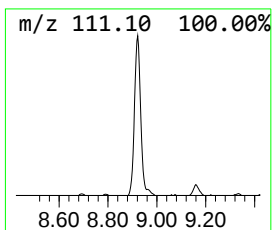
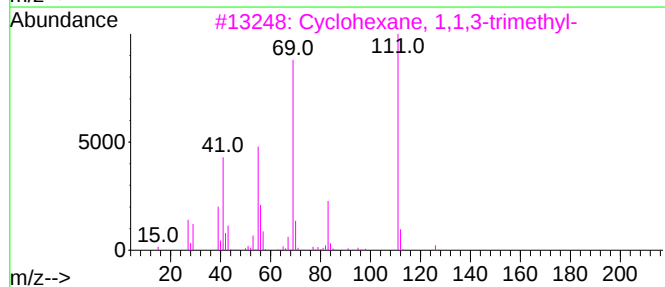
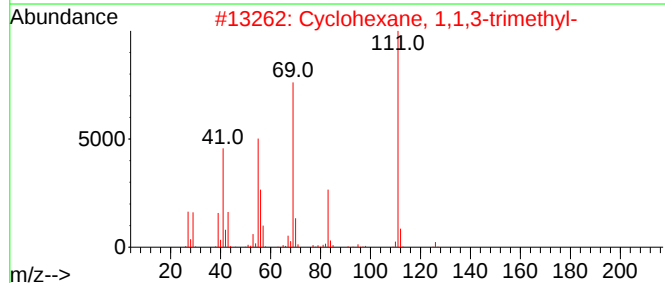
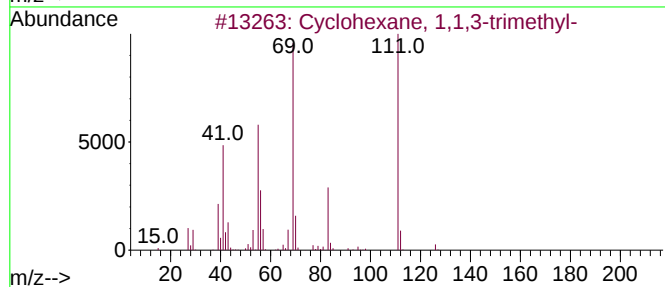
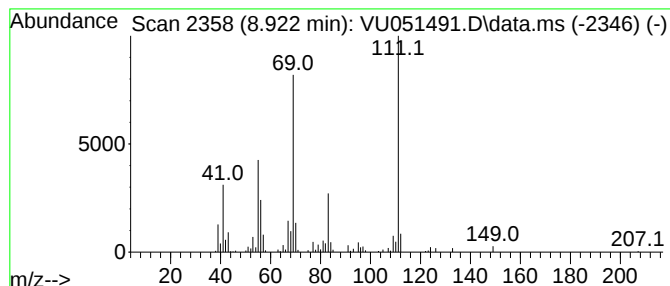
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM102022WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Cyclic8.922 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.922	7.02 ug/L	234002	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	94
2			Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	91
3			Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	90
4			Cyclohexane, 1,3,5-trimethyl-, (...)	126	C9H18	001795-26-2	72
5			Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	64



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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBLN6ME

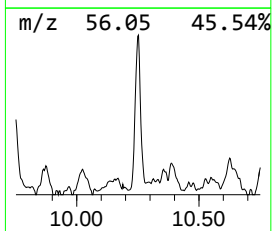
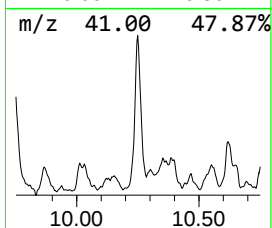
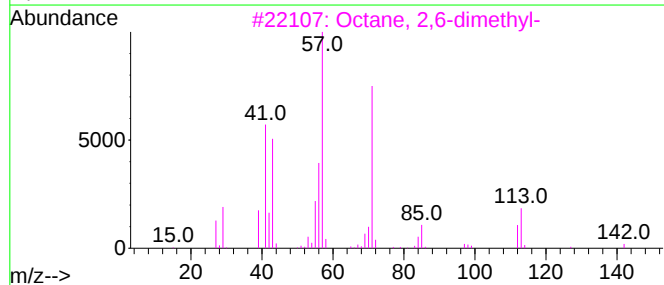
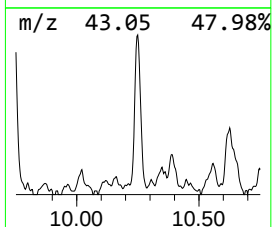
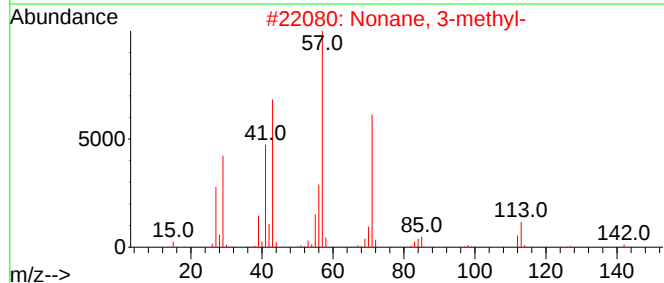
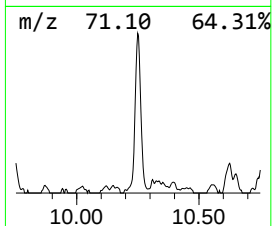
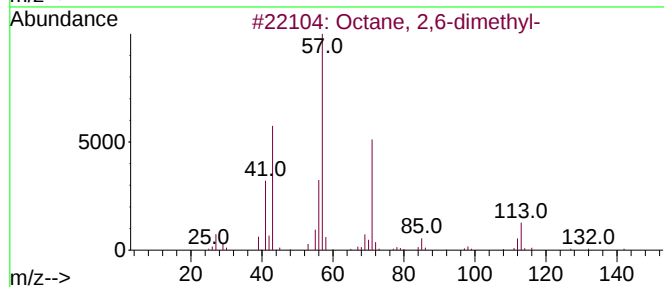
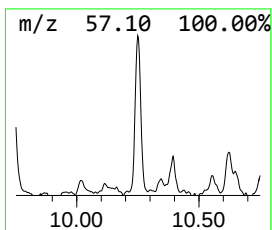
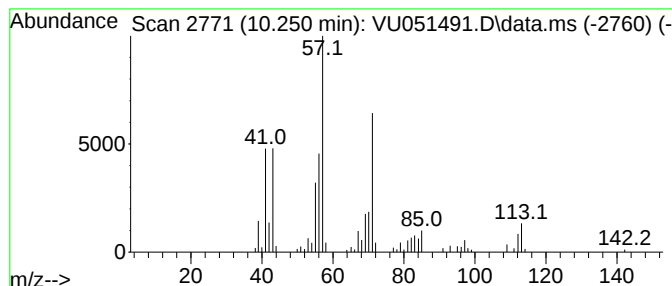
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM102022WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.250	3.13 ug/L	104472	Chlorobenzene-d5	9.420

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2,6-dimethyl-			142	C10H22	002051-30-1	86
2	Nonane, 3-methyl-			142	C10H22	005911-04-6	76
3	Octane, 2,6-dimethyl-			142	C10H22	002051-30-1	70
4	Nonane, 3-methyl-			142	C10H22	005911-04-6	68
5	Undecane, 2,6-dimethyl-			184	C13H28	017301-23-4	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102522\
Data File : VU051491.D
Acq On : 25 Oct 2022 17:15
Operator : JC/MD
Sample : N5258-07ME
Misc : 6.48g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBLN6ME

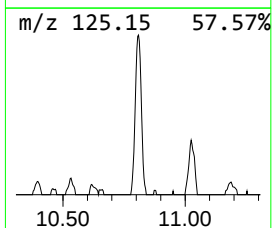
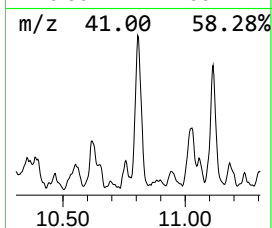
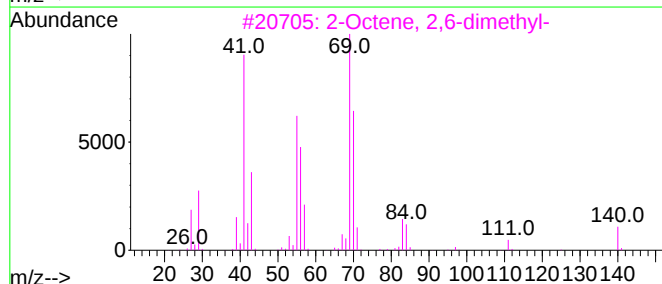
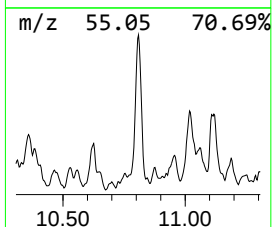
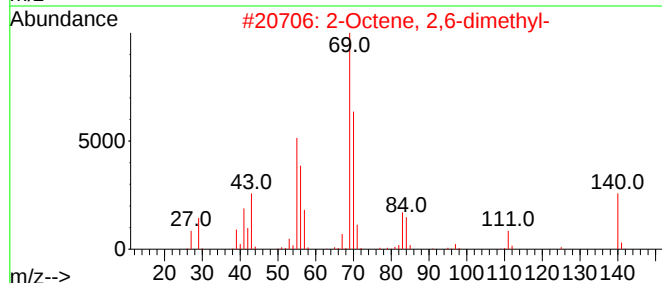
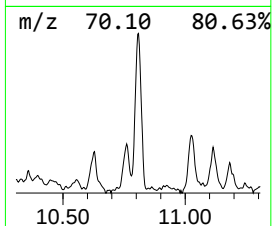
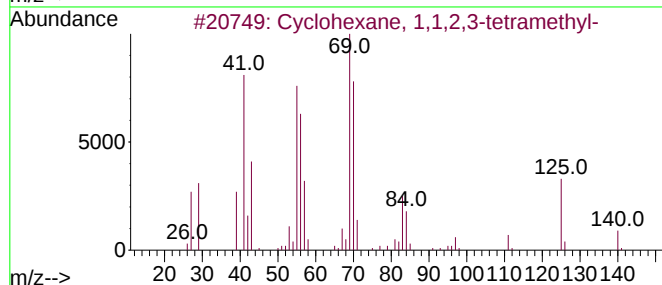
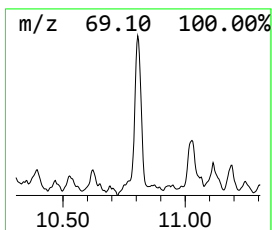
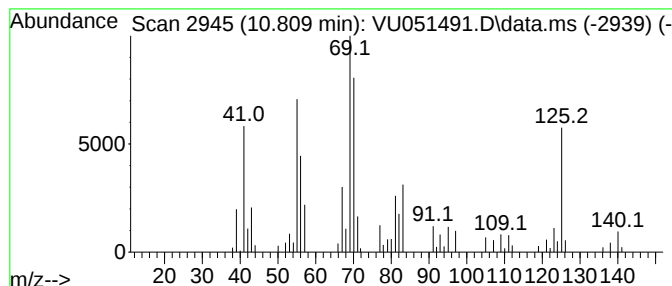
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Quant Title : VOC Analysis

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

Peak Number 6 (DEL) Alkane: Cyclic10.809 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.809	3.60 ug/L	112401	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1,1,2,3-tetramethyl-	140	C10H20	006783-92-2	62
2			2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	53
3			2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	53
4			2-Octene, 2,6-dimethyl-	140	C10H20	004057-42-5	53
5			4-Octene, 2,6-dimethyl-, [S-(E)]-	140	C10H20	062960-76-3	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102522\
Data File : VU051491.D
Acq On : 25 Oct 2022 17:15
Operator : JC/MD
Sample : N5258-07ME
Misc : 6.48g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBLN6ME

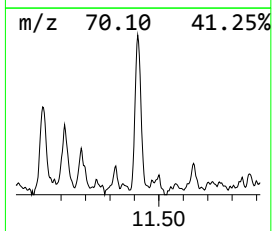
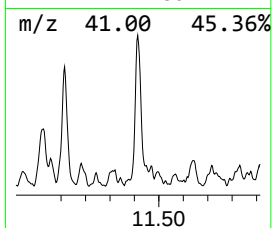
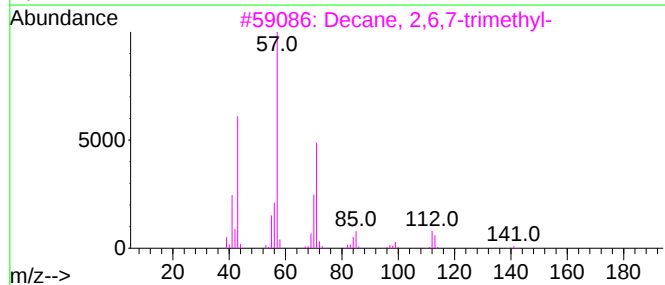
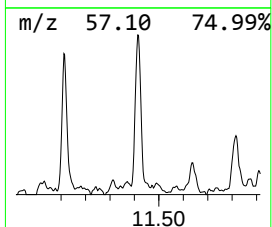
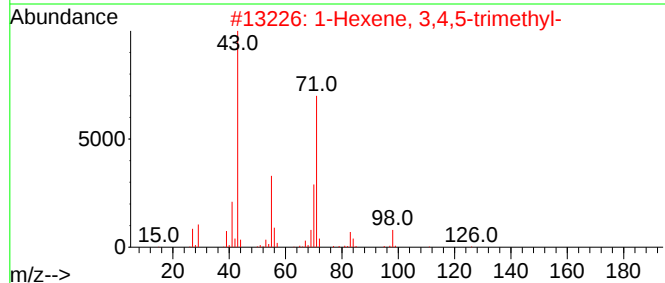
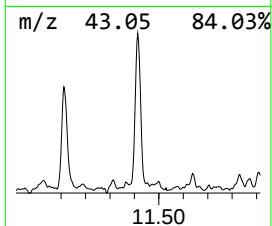
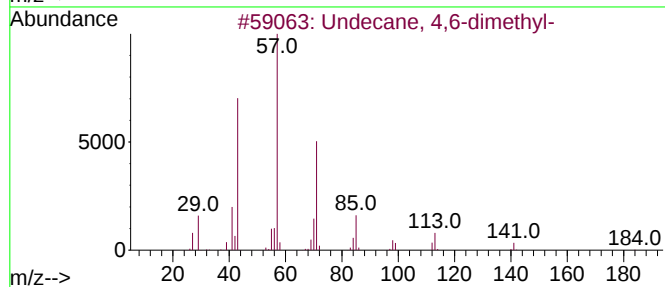
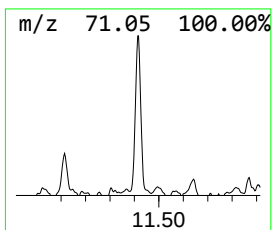
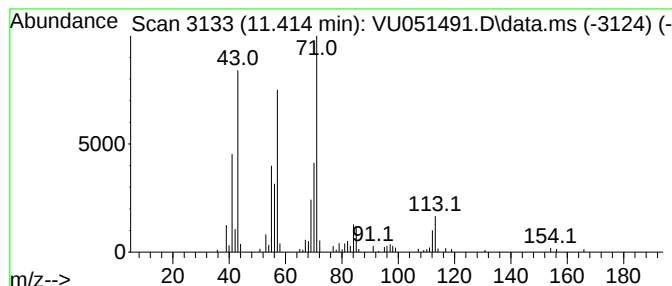
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Quant Title : VOC Analysis

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.414	3.00 ug/L	93815	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	59
2			1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	50
3			Decane, 2,6,7-trimethyl-	184	C13H28	062108-25-2	50
4			4-(Methylamino)-1-thiane-1,1-dione	163	C6H13N02S	1000444-06-6	47
5			Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102522\
Data File : VU051491.D
Acq On : 25 Oct 2022 17:15
Operator : JC/MD
Sample : N5258-07ME
Misc : 6.48g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBLN6ME

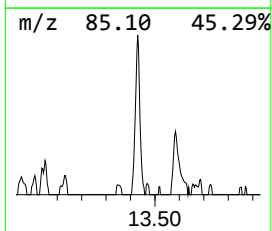
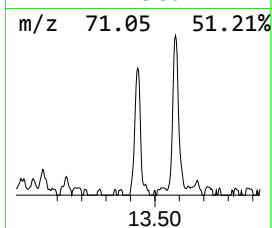
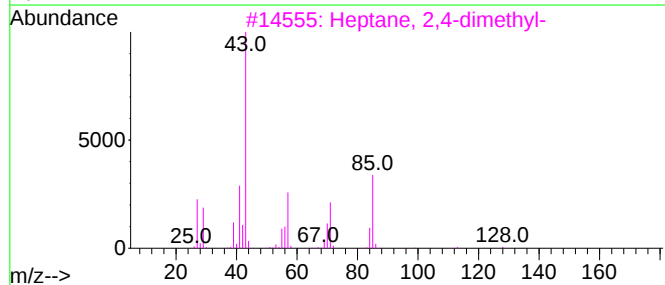
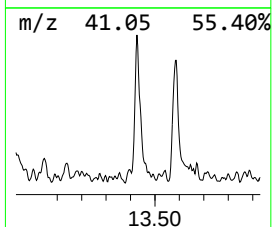
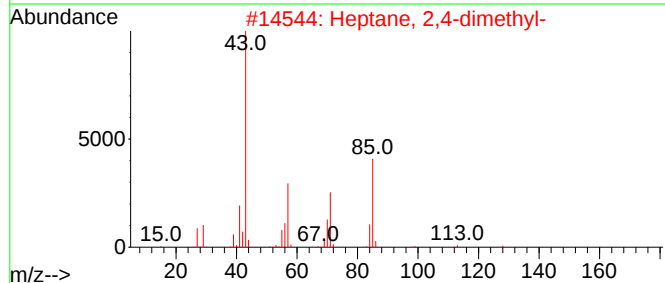
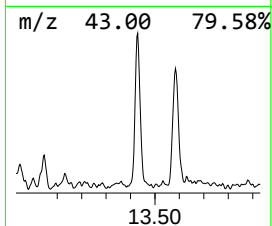
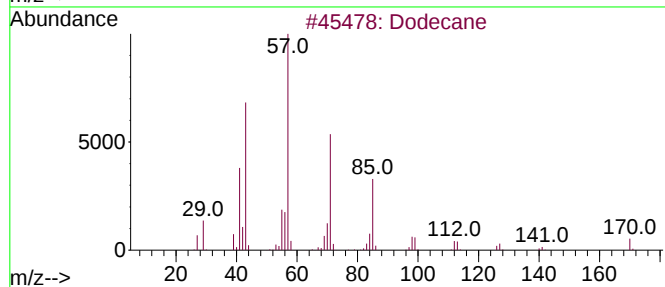
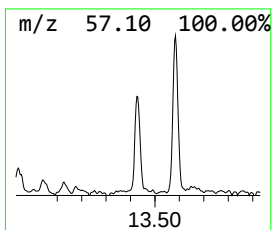
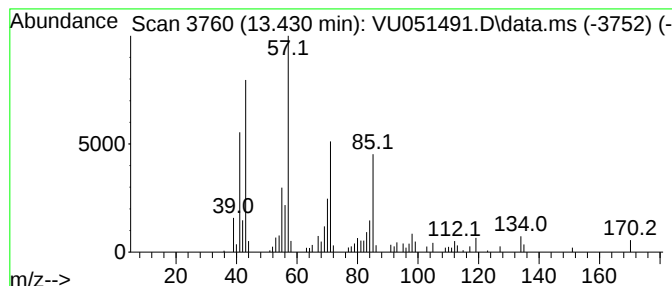
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM102022WMA.M
Quant Title : VOC Analysis

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.430	2.70 ug/L	84449	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	83
2			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	72
3			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	72
4			Silane, trichlorooctadecyl-	386	C18H37Cl3Si	000112-04-9	64
5			Octane	114	C8H18	000111-65-9	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102522\
Data File : VU051491.D
Acq On : 25 Oct 2022 17:15
Operator : JC/MD
Sample : N5258-07ME
Misc : 6.48g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
GBLN6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM102022WMA.M
Quant Title : VOC Analysis

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

						--Internal Standard--			
TIC Top	Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(DEL)	Alkane: S...	7.494	2.6	ug/L	67175	1	6.243	1300780	50.0
(DEL)	Alkane: C...	8.922	7.0	ug/L	234002	2	9.420	1666670	50.0
(DEL)	Alkane: S...	10.250	3.1	ug/L	104472	2	9.420	1666670	50.0
(DEL)	Alkane: C...	10.809	3.6	ug/L	112401	3	11.812	1563120	50.0
(DEL)	Alkane: S...	11.414	3.0	ug/L	93815	3	11.812	1563120	50.0
(DEL)	Alkane: S...	13.430	2.7	ug/L	84449	3	11.812	1563120	50.0