

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
 Data File : VU045294.D
 Acq On : 12 Oct 2021 16:10
 Operator : SY/MD
 Sample : M4070-09ME
 Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW7E6ME

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\SFAMULM092321WMA.M

Title : VOC Analysis

Signal : TIC: VU045294.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.459	30	37	42	rBV	32735	43898	3.45%	0.328%
2	1.597	73	80	93	rVB	101708	128088	10.06%	0.956%
3	1.871	160	165	176	rVB	41562	49178	3.86%	0.367%
4	1.928	178	183	191	rVB	27955	29779	2.34%	0.222%
5	2.523	355	368	387	rBV	187138	334001	26.24%	2.492%
6	2.613	388	396	423	rVB	6897	20735	1.63%	0.155%
7	2.748	428	438	452	rVB	4998	8060	0.63%	0.060%
8	3.002	494	517	519	rBV4	10146	24228	1.90%	0.181%
9	3.324	597	617	632	rBV2	22858	50067	3.93%	0.374%
10	3.668	713	724	736	rVB2	4505	8795	0.69%	0.066%
11	4.407	944	954	955	rBV4	2008	2617	0.21%	0.020%
12	4.510	969	986	1004	rVB2	49612	122021	9.59%	0.910%
13	4.649	1013	1029	1070	rBV	113305	363376	28.55%	2.711%
14	5.063	1140	1158	1183	rBV	208438	488724	38.40%	3.646%
15	5.372	1237	1254	1268	rVV5	47480	118080	9.28%	0.881%
16	5.449	1269	1278	1298	rVB3	10837	23370	1.84%	0.174%
17	5.578	1307	1318	1329	rBV3	13754	29815	2.34%	0.222%
18	5.719	1342	1362	1387	rBV2	497658	1272767	100.00%	9.496%
19	5.841	1388	1400	1411	rVV4	27535	56986	4.48%	0.425%
20	5.912	1411	1422	1432	rVV2	23939	47586	3.74%	0.355%
21	5.980	1432	1443	1459	rVB2	49823	105424	8.28%	0.787%
22	6.124	1477	1488	1499	rBV2	8445	15751	1.24%	0.118%
23	6.250	1511	1527	1547	rBV	346266	693816	54.51%	5.177%
24	6.526	1604	1613	1624	rVV5	4174	7711	0.61%	0.058%
25	6.603	1627	1637	1650	rVV2	3921	8821	0.69%	0.066%
26	6.693	1650	1665	1676	rVV	293792	612260	48.10%	4.568%
27	6.758	1677	1685	1708	rVV2	197983	398858	31.34%	2.976%
28	6.857	1708	1716	1726	rVB8	2212	4509	0.35%	0.034%
29	6.976	1742	1753	1765	rVB4	15987	29821	2.34%	0.222%
30	7.070	1769	1782	1793	rVB	19193	35275	2.77%	0.263%
31	7.189	1810	1819	1821	rBV5	4114	5317	0.42%	0.040%
32	7.230	1825	1832	1845	rVB4	20094	38230	3.00%	0.285%
33	7.430	1884	1894	1900	rBV3	2487	4470	0.35%	0.033%
34	7.497	1900	1915	1924	rBV3	14338	28784	2.26%	0.215%
35	7.571	1925	1938	1957	rVB	147496	283549	22.28%	2.116%
36	7.655	1958	1964	1973	rBV4	4267	6142	0.48%	0.046%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
 Data File : VU045294.D
 Acq On : 12 Oct 2021 16:10
 Operator : SY/MD
 Sample : M4070-09ME
 Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW7E6ME

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\SFAMULM092321WMA.M
 Title : VOC Analysis

37	7.857	2013	2027	2028	rBV2	23171	30104	2.37%	0.225%
38	7.899	2030	2040	2054	rVB	548257	1007385	79.15%	7.516%
39	7.973	2054	2063	2072	rBV	57639	99202	7.79%	0.740%
40	8.185	2119	2129	2140	rBV	95103	182128	14.31%	1.359%
41	8.369	2175	2186	2196	rBV4	7889	14188	1.11%	0.106%
42	8.478	2212	2220	2228	rVB6	3288	5206	0.41%	0.039%
43	8.549	2228	2242	2257	rVB8	2452	5166	0.41%	0.039%
44	8.652	2257	2274	2299	rBV	418879	804339	63.20%	6.001%
45	8.809	2315	2323	2331	rVB6	9330	14354	1.13%	0.107%
46	8.864	2331	2340	2350	rVB	29253	47437	3.73%	0.354%
47	8.928	2350	2360	2368	rBV2	20435	35756	2.81%	0.267%
48	9.073	2395	2405	2413	rBV3	6608	11028	0.87%	0.082%
49	9.124	2413	2421	2428	rVV2	8066	12436	0.98%	0.093%
50	9.166	2428	2434	2442	rVB4	6835	9344	0.73%	0.070%
51	9.217	2442	2450	2459	rVB4	6120	10311	0.81%	0.077%
52	9.336	2480	2487	2501	rVB3	5770	9658	0.76%	0.072%
53	9.426	2501	2515	2532	rBV	479132	865066	67.97%	6.454%
54	9.513	2535	2542	2550	rVB2	11011	17114	1.34%	0.128%
55	9.578	2550	2562	2574	rVB	58530	99173	7.79%	0.740%
56	9.700	2574	2600	2610	rBV	115570	228440	17.95%	1.704%
57	9.880	2648	2656	2668	rVB8	1552	3227	0.25%	0.024%
58	10.041	2690	2706	2714	rBV6	5895	15362	1.21%	0.115%
59	10.108	2714	2727	2742	rVB	131064	219845	17.27%	1.640%
60	10.250	2758	2771	2773	rBV5	17261	26999	2.12%	0.201%
61	10.362	2796	2806	2813	rBV4	16887	32482	2.55%	0.242%
62	10.491	2834	2846	2855	rBV	44271	70795	5.56%	0.528%
63	10.533	2855	2859	2863	rBV5	2568	2719	0.21%	0.020%
64	10.629	2879	2889	2892	rBV6	2571	4241	0.33%	0.032%
65	10.764	2919	2931	2944	rBV	456113	744303	58.48%	5.553%
66	10.912	2967	2977	2986	rBV	60653	91911	7.22%	0.686%
67	11.005	2996	3006	3021	rVB	46098	95206	7.48%	0.710%
68	11.118	3029	3041	3057	rVB3	25302	62689	4.93%	0.468%
69	11.298	3087	3097	3113	rVV	36182	59442	4.67%	0.443%
70	11.420	3127	3135	3141	rBV2	15254	21730	1.71%	0.162%
71	11.471	3142	3151	3173	rVB	81314	139413	10.95%	1.040%
72	11.616	3179	3196	3199	rBV2	8856	16507	1.30%	0.123%
73	11.648	3200	3206	3216	rVB2	21894	33855	2.66%	0.253%
74	11.819	3246	3259	3272	rBV	541220	853788	67.08%	6.370%
75	11.899	3274	3284	3296	rVB	38776	66592	5.23%	0.497%
76	12.102	3338	3347	3350	rBV4	10253	14750	1.16%	0.110%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
 Data File : VU045294.D
 Acq On : 12 Oct 2021 16:10
 Operator : SY/MD
 Sample : M4070-09ME
 Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW7E6ME

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\SFAMULM092321WMA.M
 Title : VOC Analysis

77	12.198	3364	3377	3397	rVB	596672	966458	75.93%	7.211%
78	12.330	3411	3418	3427	rVV2	27136	38653	3.04%	0.288%
79	12.381	3428	3434	3448	rVB	15313	26937	2.12%	0.201%
80	12.471	3454	3462	3467	rBV	14797	22091	1.74%	0.165%
81	12.574	3490	3494	3501	rVB	7585	8615	0.68%	0.064%
82	12.774	3550	3556	3562	rBV7	3269	4687	0.37%	0.035%
83	12.877	3583	3588	3597	rVB4	6758	10109	0.79%	0.075%
84	13.111	3655	3661	3664	rBV4	4293	4906	0.39%	0.037%
85	13.359	3732	3738	3745	rBV7	3712	4695	0.37%	0.035%
86	13.436	3754	3762	3781	rVB5	24899	57205	4.49%	0.427%
87	13.590	3799	3810	3818	rBV2	11695	18284	1.44%	0.136%
88	13.738	3847	3856	3863	rBV10	3867	7073	0.56%	0.053%
89	13.838	3878	3887	3897	rBV5	11499	19929	1.57%	0.149%
90	14.089	3944	3965	3983	rBV	145500	250228	19.66%	1.867%
91	14.195	3990	3998	4011	rVB2	15183	24177	1.90%	0.180%
92	14.452	4071	4078	4091	rVV2	14955	23564	1.85%	0.176%
93	14.520	4093	4099	4108	rVB8	9438	14973	1.18%	0.112%
94	14.674	4135	4147	4156	rVB10	3139	6450	0.51%	0.048%
95	15.227	4307	4319	4329	rBV	79929	133117	10.46%	0.993%
96	15.413	4361	4377	4394	rBV	73938	131226	10.31%	0.979%
97	15.500	4399	4404	4412	rVB9	2210	3417	0.27%	0.025%
98	16.185	4614	4617	4629	rVB8	4937	6751	0.53%	0.050%
99	16.265	4632	4642	4649	rBV4	6253	12095	0.95%	0.090%
100	16.413	4680	4688	4694	rBV3	14336	22824	1.79%	0.170%

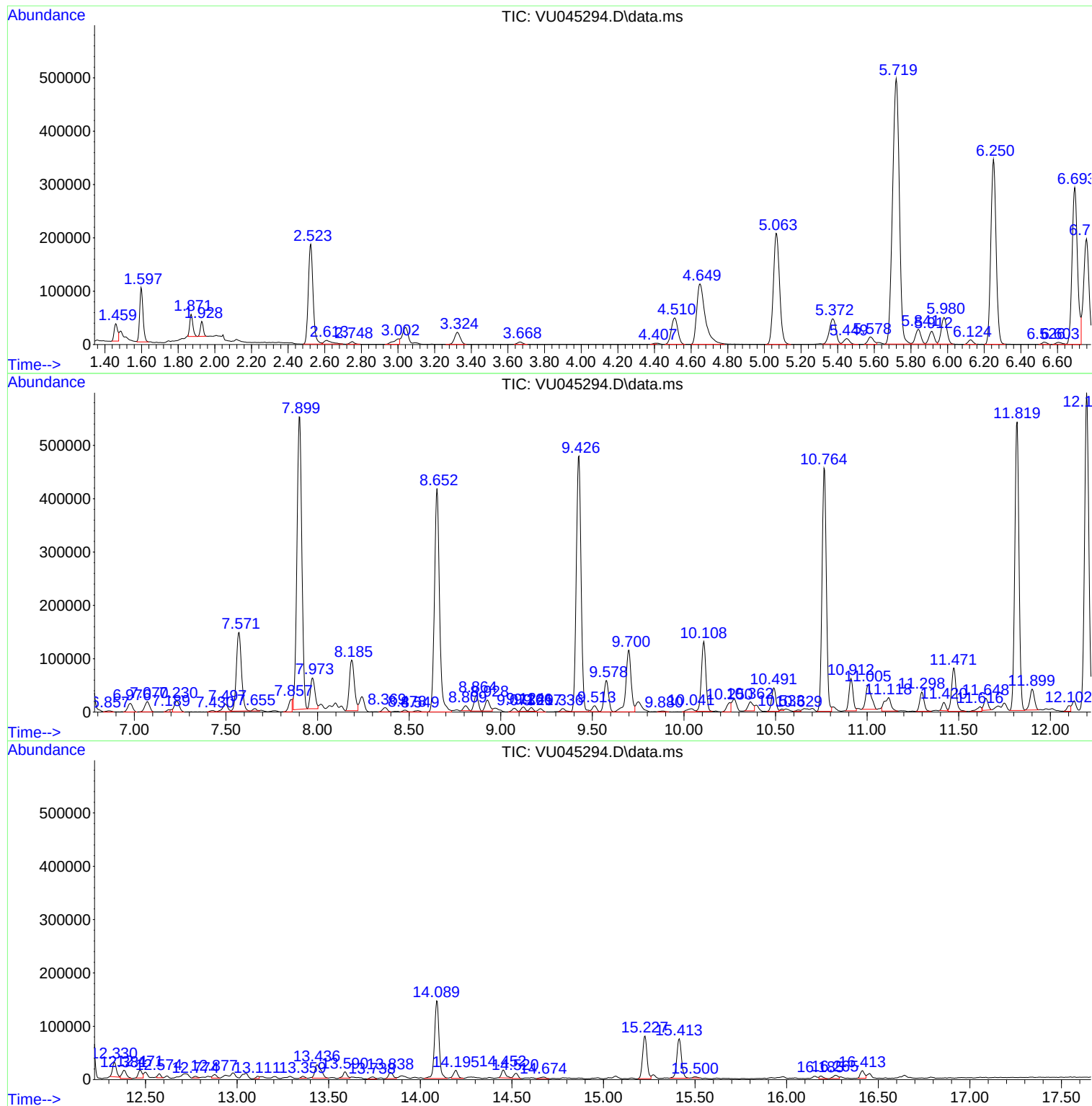
Sum of corrected areas: 13403064

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
Data File : VU045294.D
Acq On : 12 Oct 2021 16:10
Operator : SY/MD
Sample : M4070-09ME
Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
Data File : VU045294.D
Acq On : 12 Oct 2021 16:10
Operator : SY/MD
Sample : M4070-09ME
Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E6ME

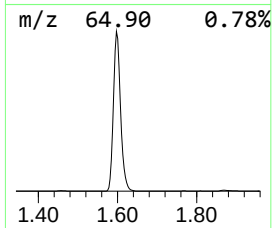
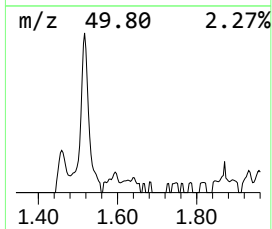
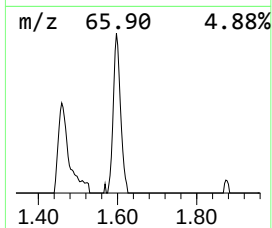
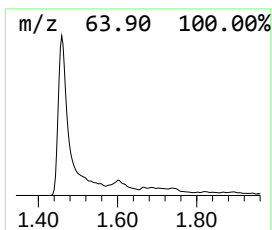
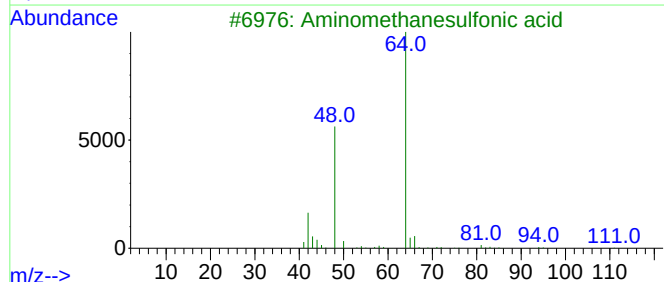
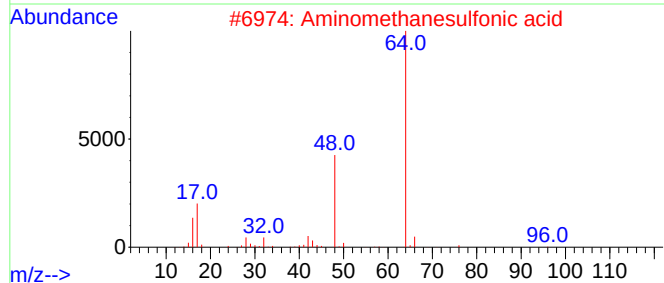
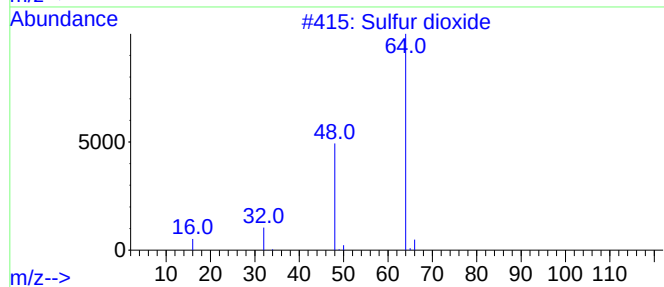
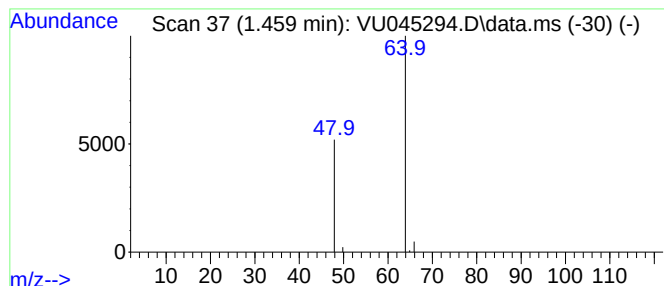
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.459	3.16 ug/L	43898	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
Data File : VU045294.D
Acq On : 12 Oct 2021 16:10
Operator : SY/MD
Sample : M4070-09ME
Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E6ME

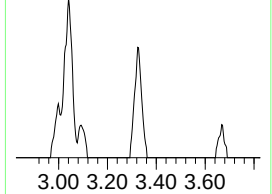
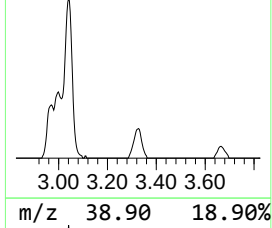
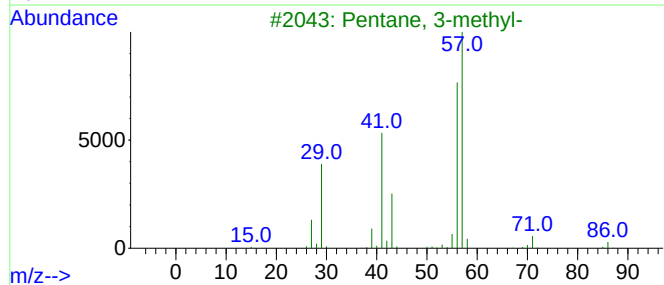
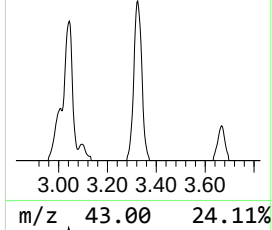
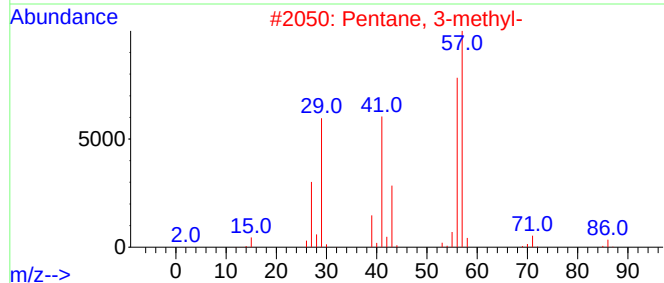
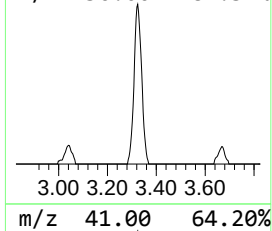
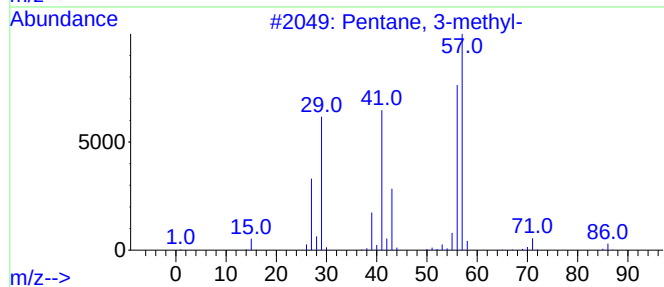
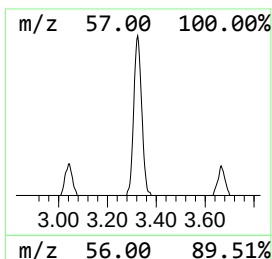
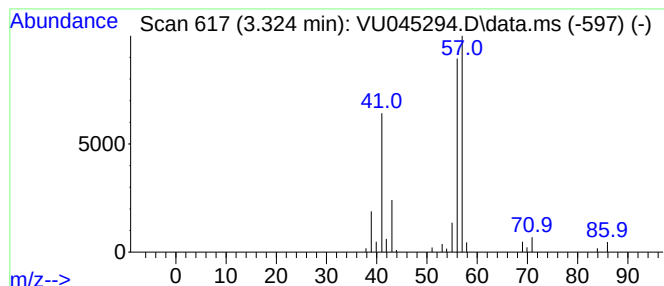
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.324	3.61 ug/L	50067	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2			Pentane, 3-methyl-	86	C6H14	000096-14-0	90
3			Pentane, 3-methyl-	86	C6H14	000096-14-0	86
4			Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	83
5			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	78



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
Data File : VU045294.D
Acq On : 12 Oct 2021 16:10
Operator : SY/MD
Sample : M4070-09ME
Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E6ME

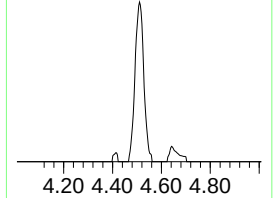
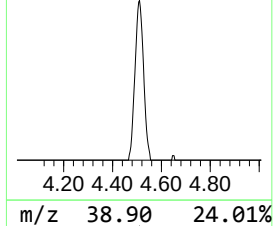
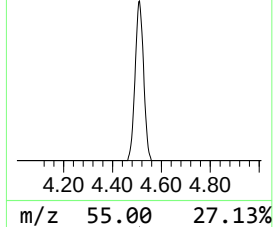
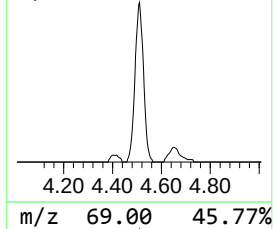
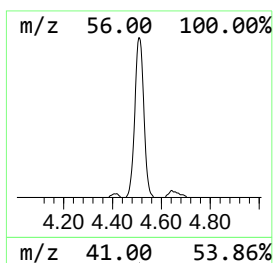
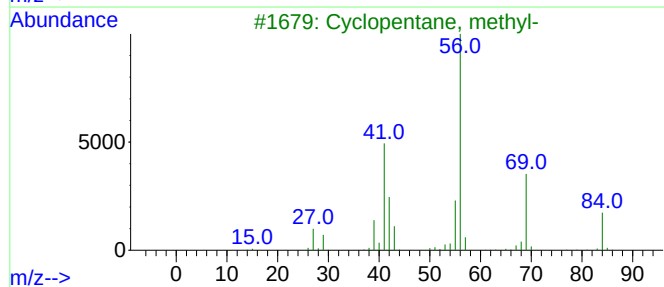
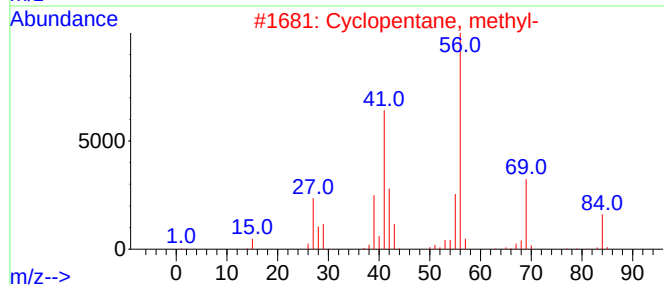
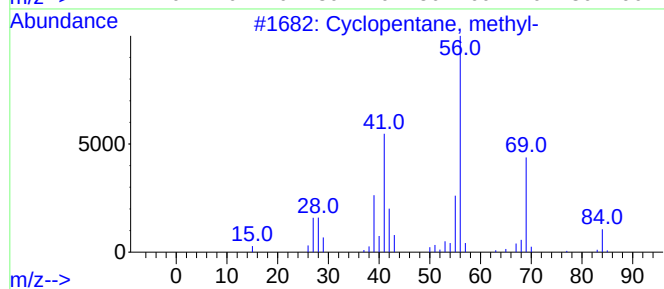
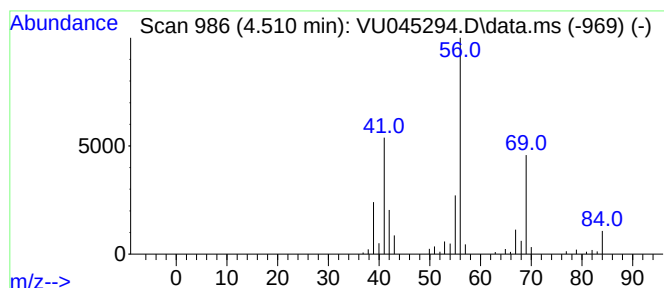
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 (DEL) Alkane: Cyclic4.510 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.510	8.79 ug/L	122021	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	86
3			Cyclopentane, methyl-	84	C6H12	000096-37-7	80
4			Cyclopentane, methyl-	84	C6H12	000096-37-7	72
5			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
Data File : VU045294.D
Acq On : 12 Oct 2021 16:10
Operator : SY/MD
Sample : M4070-09ME
Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E6ME

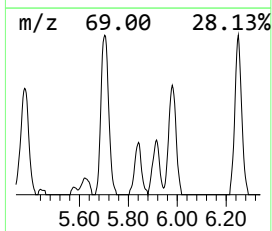
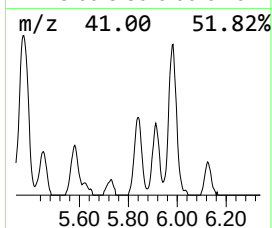
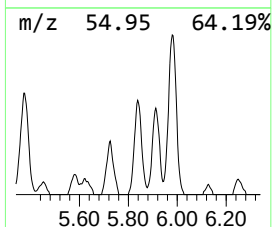
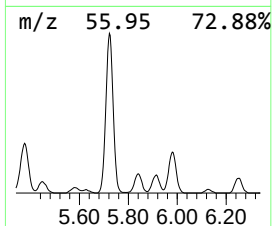
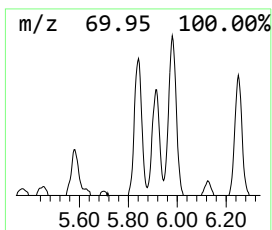
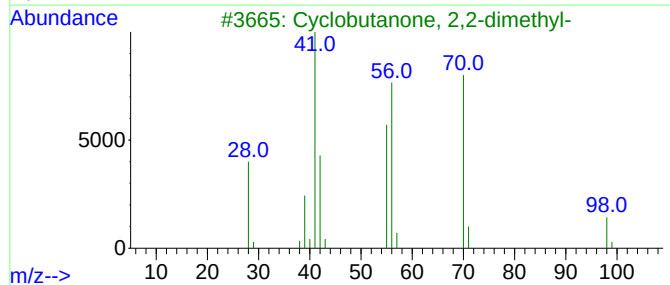
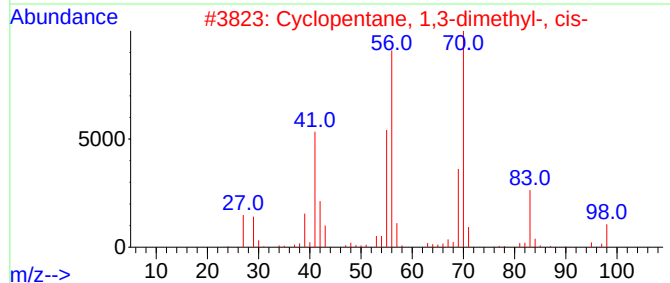
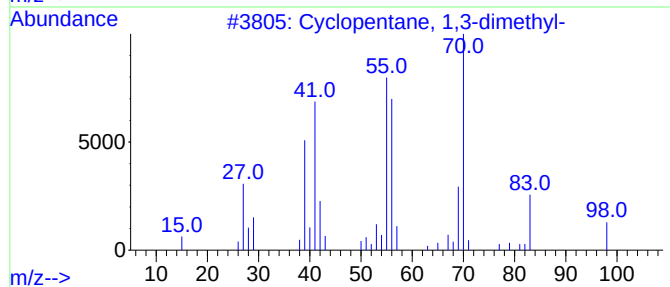
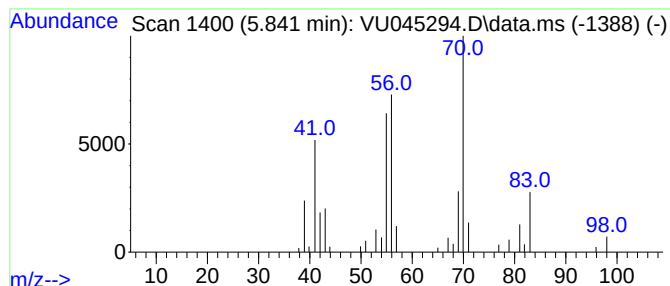
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 (DEL) Alkane: Cyclic5.841 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.841	4.11 ug/L	56986	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	90
2			Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	72
3			Cyclobutanone, 2,2-dimethyl-	98	C6H10O	001192-14-9	64
4			1-Pentene, 3,4-dimethyl-	98	C7H14	007385-78-6	64
5			Isopropylcyclobutane	98	C7H14	000872-56-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
Data File : VU045294.D
Acq On : 12 Oct 2021 16:10
Operator : SY/MD
Sample : M4070-09ME
Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E6ME

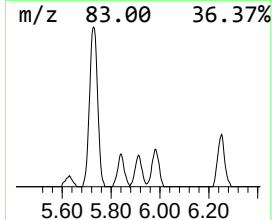
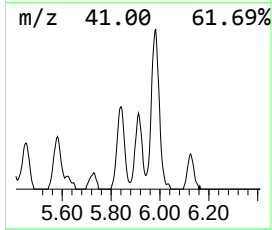
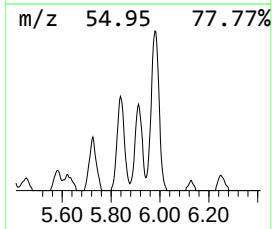
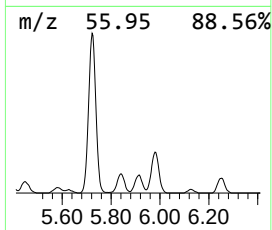
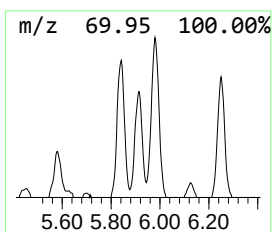
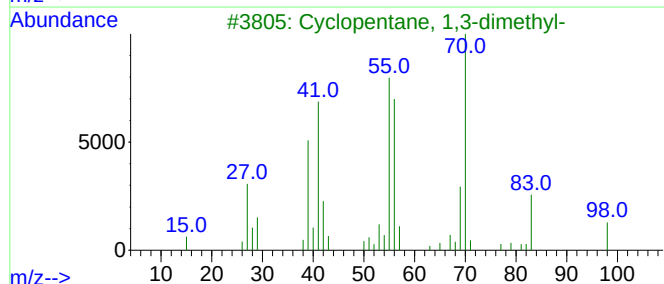
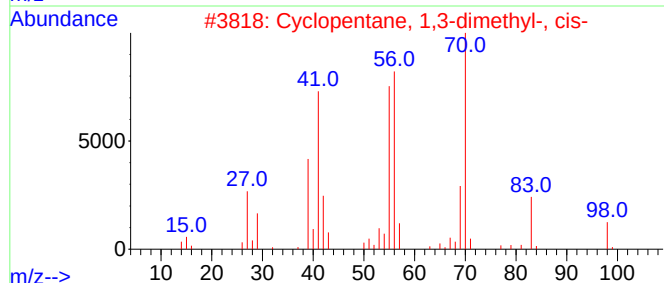
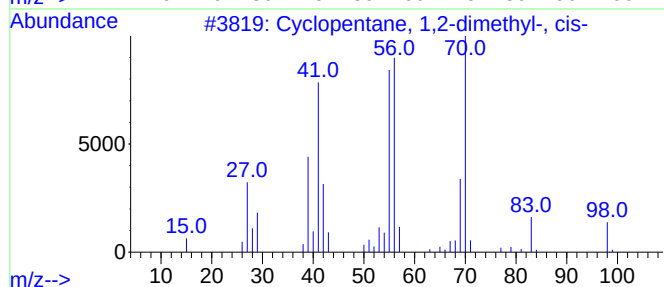
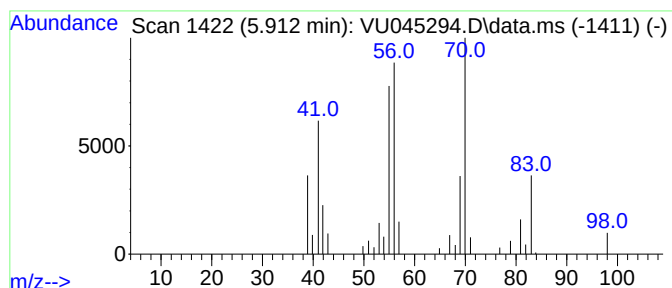
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 (DEL) Alkane: Cyclic5.912 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.912	3.43 ug/L	47586	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	93
2			Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	91
3			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	91
4			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	90
5			Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
Data File : VU045294.D
Acq On : 12 Oct 2021 16:10
Operator : SY/MD
Sample : M4070-09ME
Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E6ME

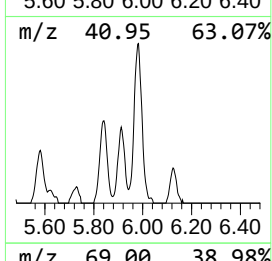
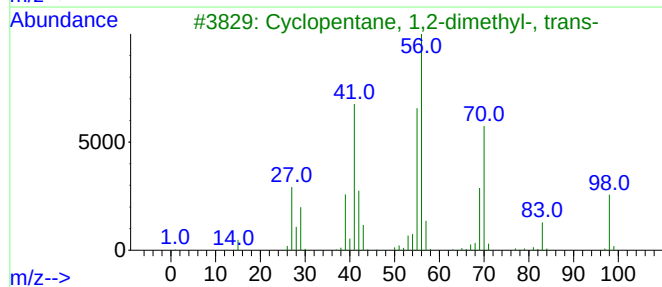
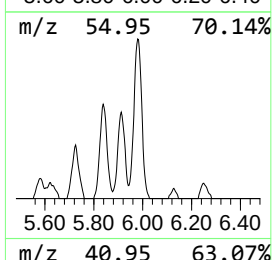
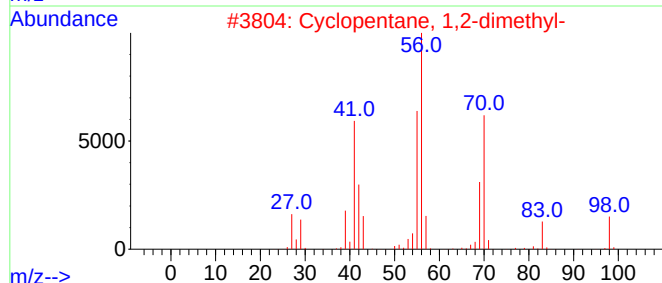
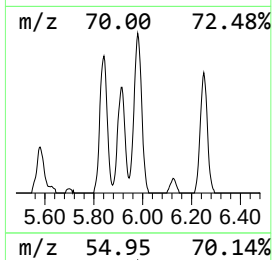
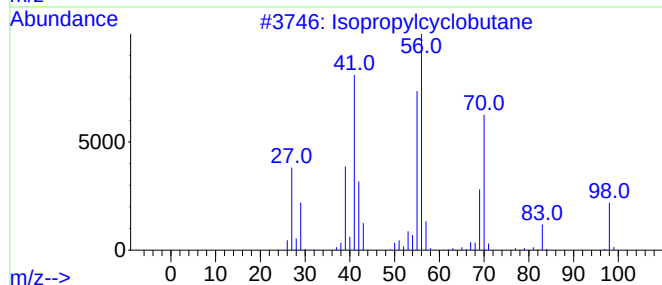
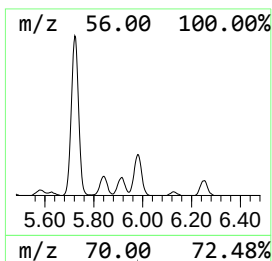
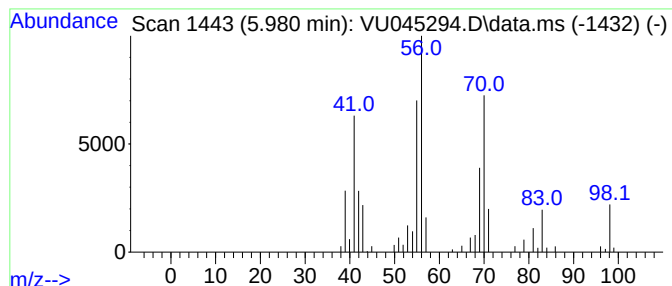
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 6 (DEL) Alkane: Cyclic5.980 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.980	7.60 ug/L	105424	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropylcyclobutane	98	C7H14	000872-56-0	91
2			Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	90
3			Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	87
4			Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	81
5			Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
Data File : VU045294.D
Acq On : 12 Oct 2021 16:10
Operator : SY/MD
Sample : M4070-09ME
Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E6ME

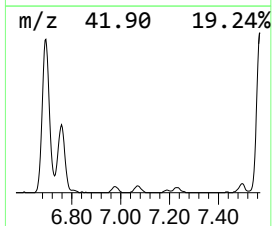
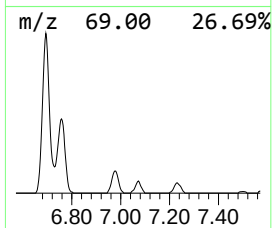
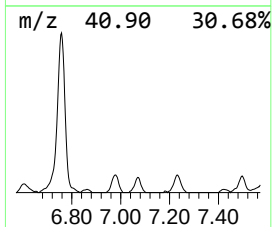
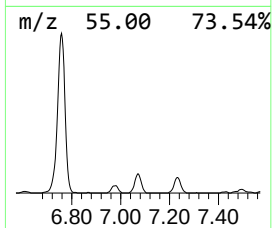
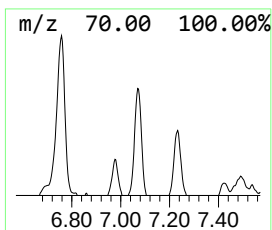
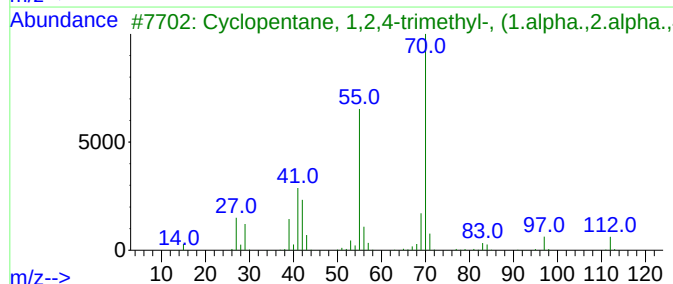
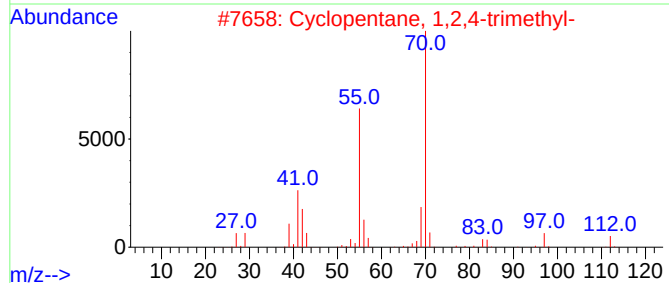
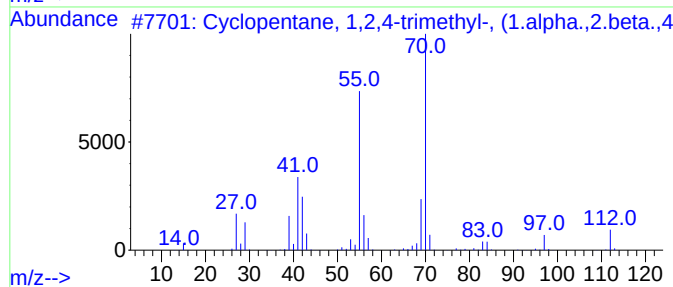
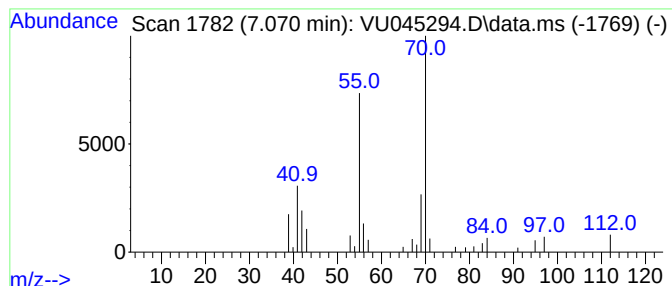
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 7 (DEL) Alkane: Cyclic7.070 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.070	2.54 ug/L	35275	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,2,4-trimethyl-, ...	112	C8H16	016883-48-0	94
2			Cyclopentane, 1,2,4-trimethyl-	112	C8H16	002815-58-9	91
3			Cyclopentane, 1,2,4-trimethyl-, ...	112	C8H16	004850-28-6	91
4			Cyclopentane, 1,2,4-trimethyl-	112	C8H16	002815-58-9	87
5			Heptane, 3-methylene-	112	C8H16	001632-16-2	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
Data File : VU045294.D
Acq On : 12 Oct 2021 16:10
Operator : SY/MD
Sample : M4070-09ME
Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E6ME

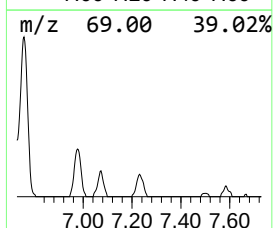
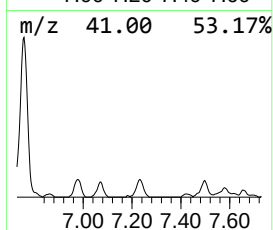
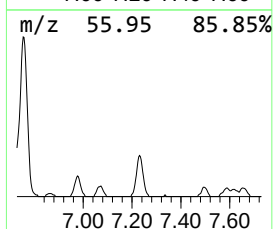
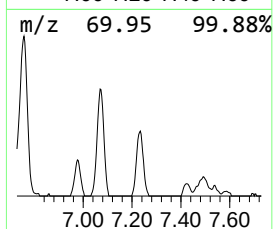
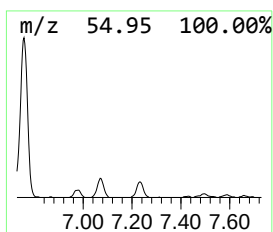
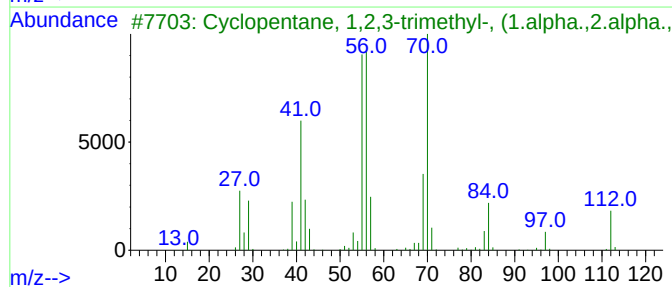
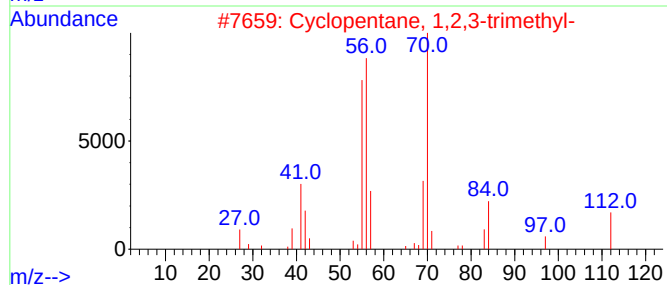
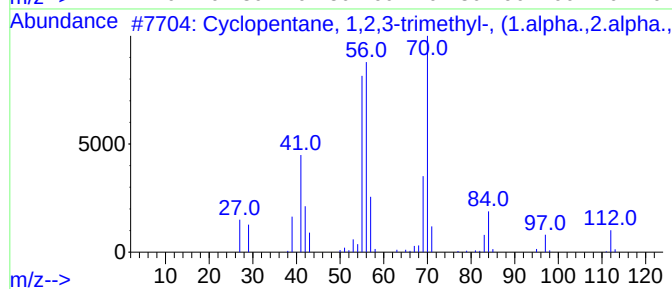
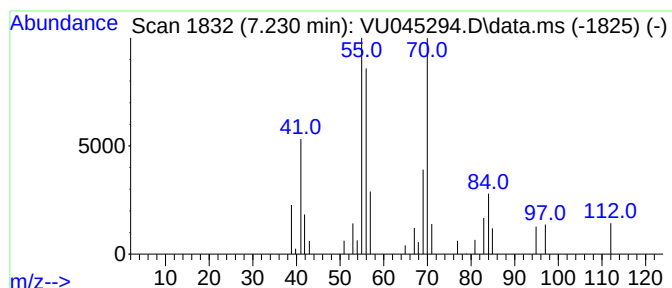
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 8 (DEL) Alkane: Cyclic7.230 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.230	2.76 ug/L	38230	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	015890-40-1	91
2			Cyclopentane, 1,2,3-trimethyl-	112	C8H16	002815-57-8	90
3			Cyclopentane, 1,2,3-trimethyl-, ...	112	C8H16	015890-40-1	90
4			Octane, 2-chloro-	148	C8H17Cl	000628-61-5	64
5			Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
Data File : VU045294.D
Acq On : 12 Oct 2021 16:10
Operator : SY/MD
Sample : M4070-09ME
Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

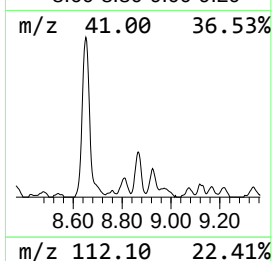
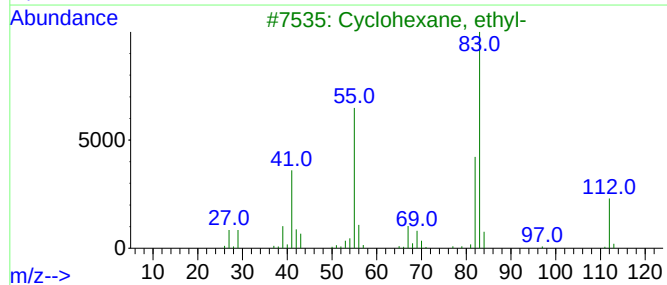
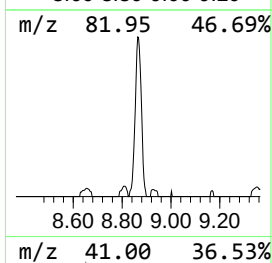
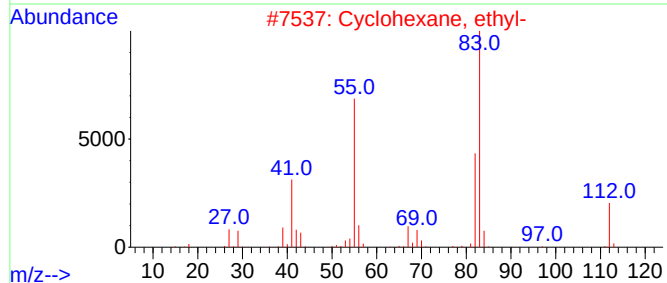
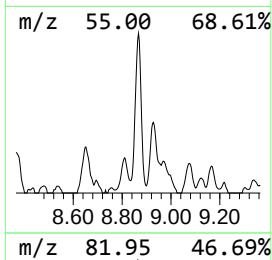
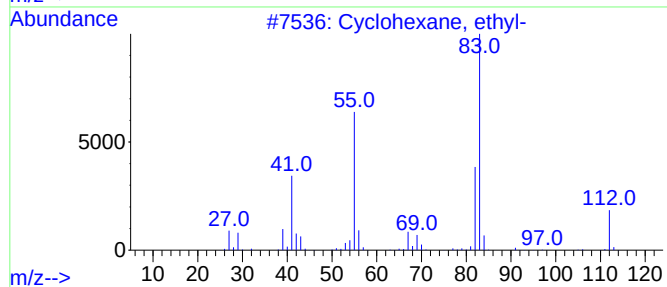
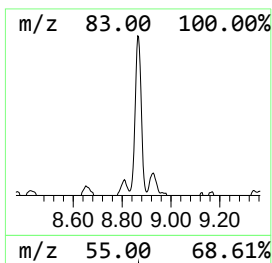
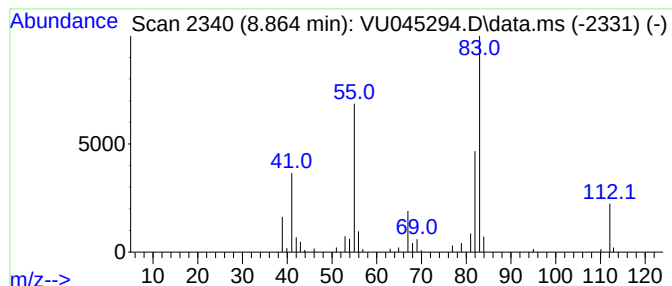
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 10 (DEL) Alkane: Cyclic8.864 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.864	2.74 ug/L	47437	Chlorobenzene-d5	9.426

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, ethyl-	112	C8H16	001678-91-7	90
2			Cyclohexane, ethyl-	112	C8H16	001678-91-7	90
3			Cyclohexane, ethyl-	112	C8H16	001678-91-7	72
4			Cyclohexane, ethyl-	112	C8H16	001678-91-7	70
5			2-Pentene, 3-ethyl-2-methyl-	112	C8H16	019780-67-7	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
Data File : VU045294.D
Acq On : 12 Oct 2021 16:10
Operator : SY/MD
Sample : M4070-09ME
Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E6ME

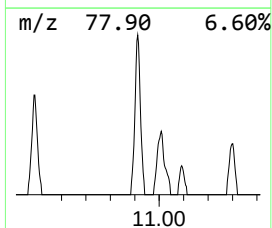
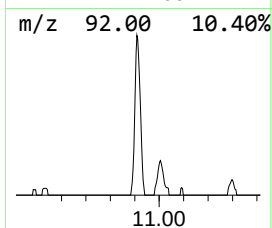
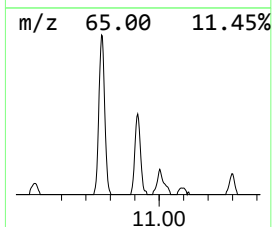
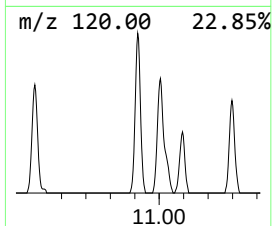
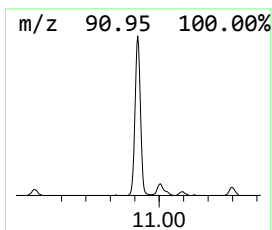
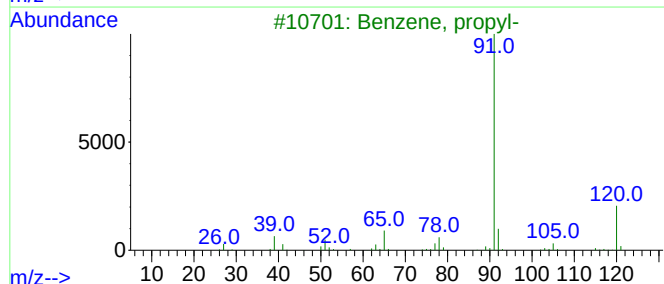
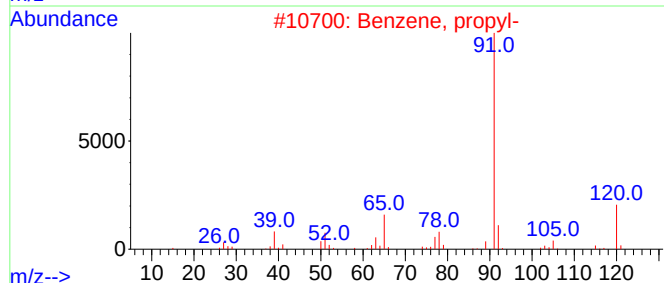
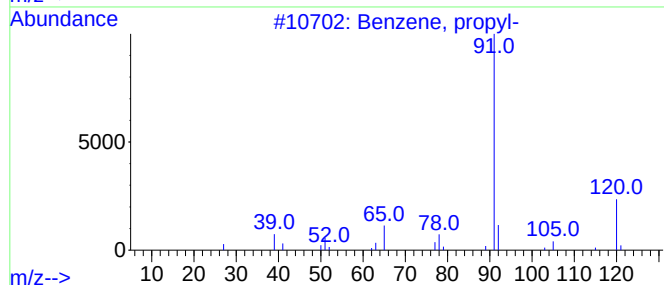
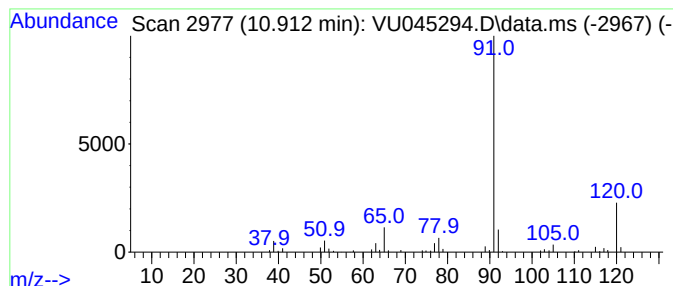
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 11 Benzene, propyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.912	5.38 ug/L	91911	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, propyl-	120	C9H12	000103-65-1	94
2			Benzene, propyl-	120	C9H12	000103-65-1	94
3			Benzene, propyl-	120	C9H12	000103-65-1	90
4			Benzene, propyl-	120	C9H12	000103-65-1	87
5			N-Benzyl-2-phenethylamine	211	C15H17N	003647-71-0	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
Data File : VU045294.D
Acq On : 12 Oct 2021 16:10
Operator : SY/MD
Sample : M4070-09ME
Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E6ME

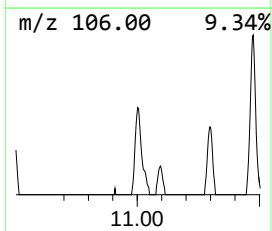
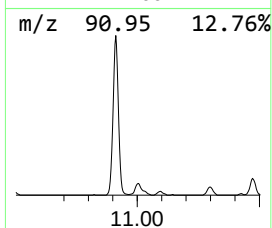
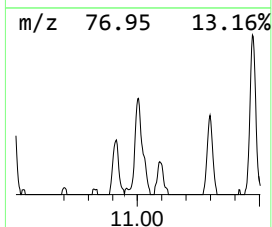
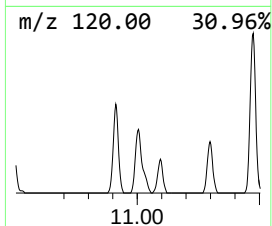
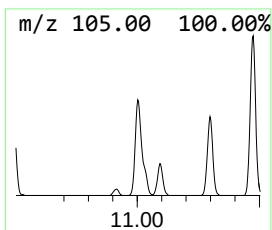
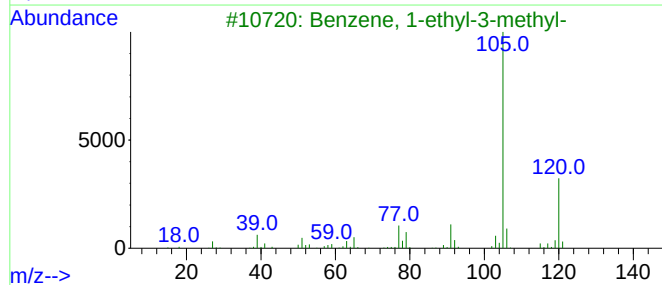
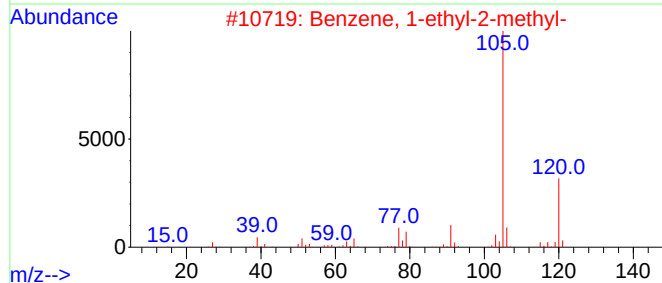
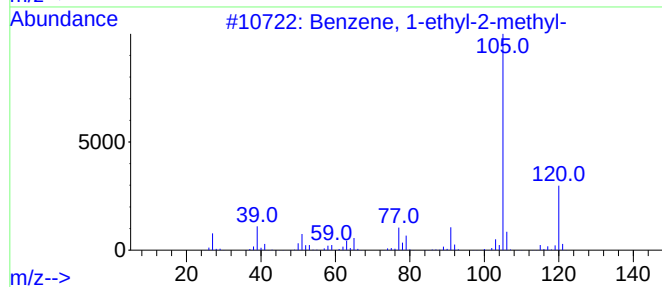
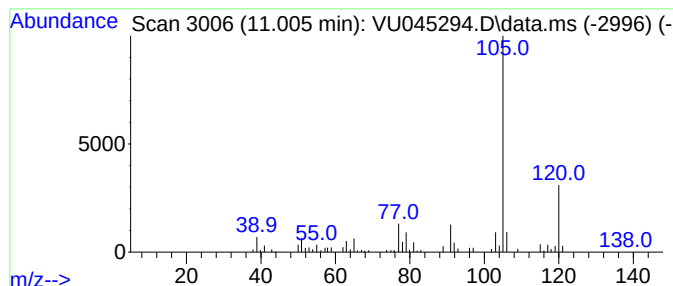
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 12 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.005	5.58 ug/L	95206	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
Data File : VU045294.D
Acq On : 12 Oct 2021 16:10
Operator : SY/MD
Sample : M4070-09ME
Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E6ME

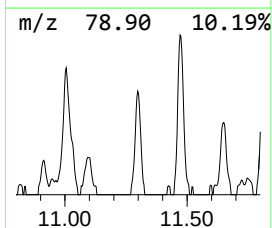
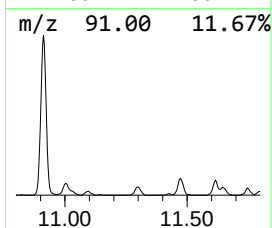
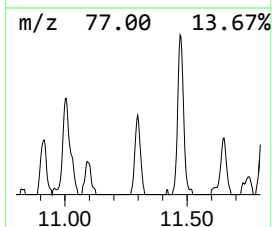
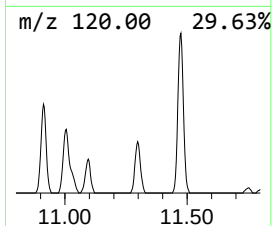
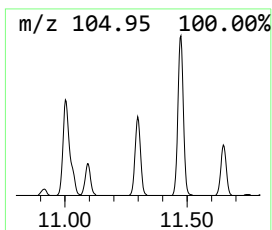
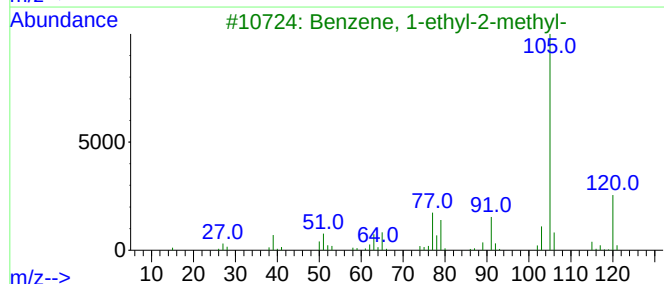
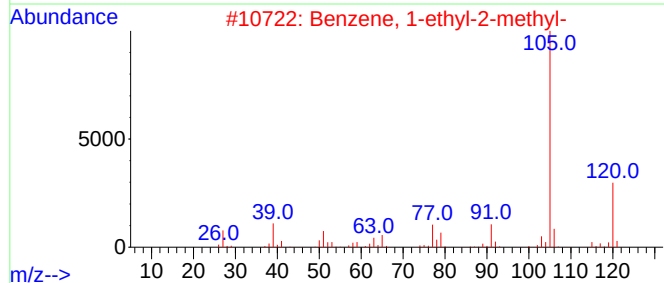
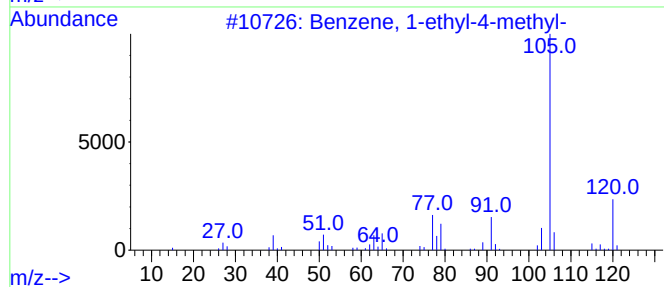
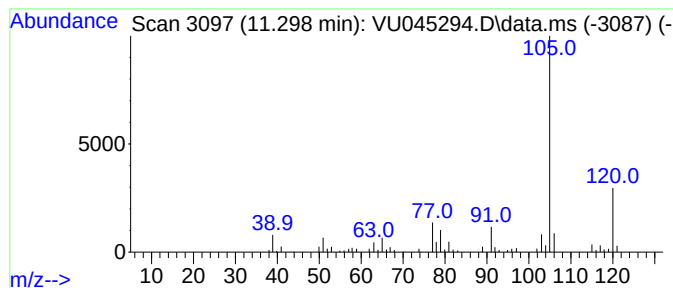
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 13 Benzene, 1-ethyl-4-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.298	3.48 ug/L	59442	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	95
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
Data File : VU045294.D
Acq On : 12 Oct 2021 16:10
Operator : SY/MD
Sample : M4070-09ME
Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E6ME

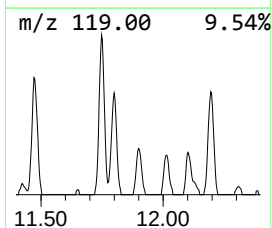
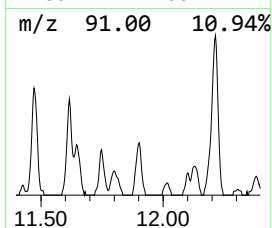
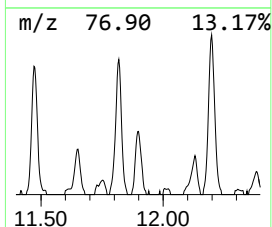
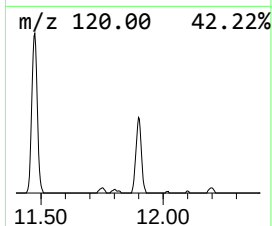
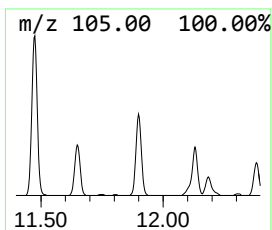
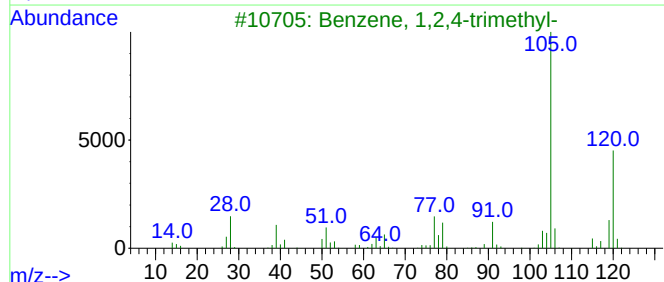
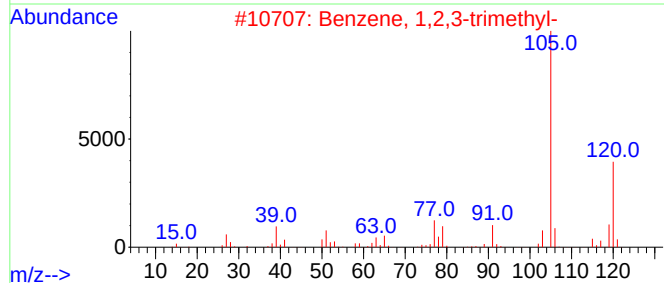
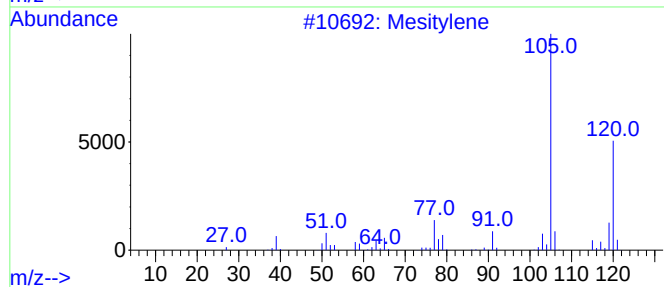
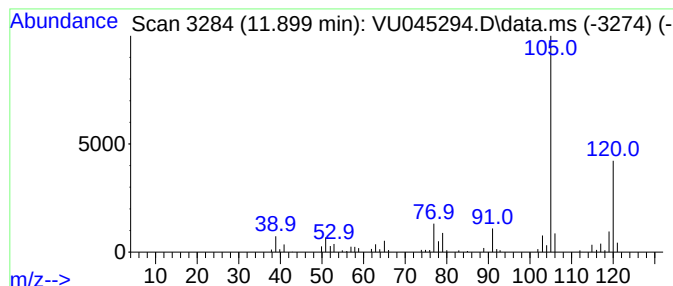
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 14 Benzene, 1,2,3-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.899	3.90 ug/L	66592	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	97
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4			Mesitylene	120	C9H12	000108-67-8	91
5			Mesitylene	120	C9H12	000108-67-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
Data File : VU045294.D
Acq On : 12 Oct 2021 16:10
Operator : SY/MD
Sample : M4070-09ME
Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E6ME

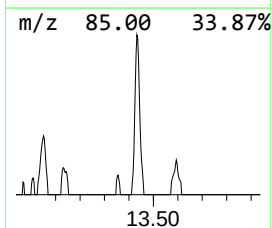
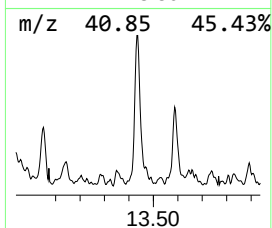
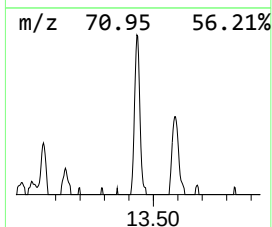
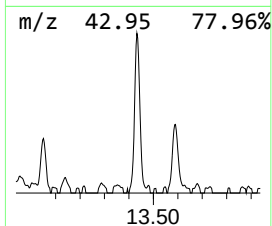
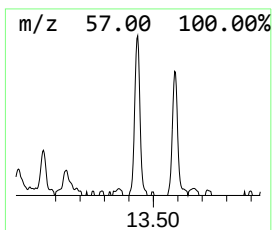
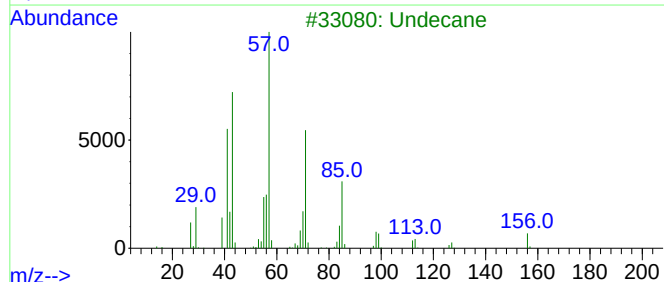
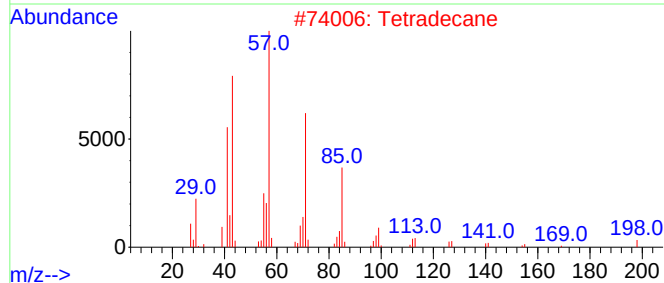
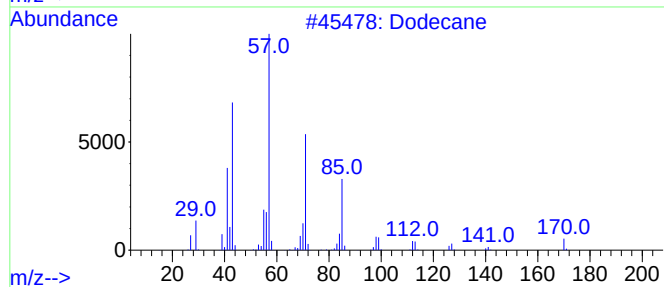
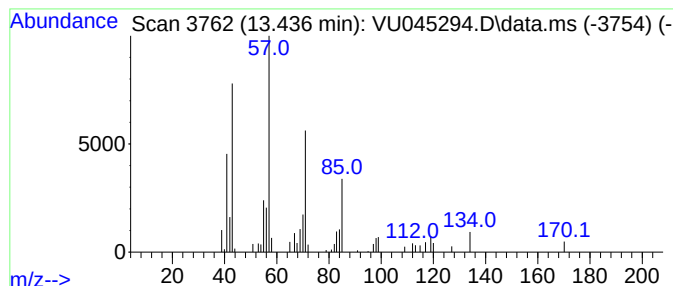
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 15 (DEL) Alkane: Straight-Chai... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.436	3.35 ug/L	57205	1,4-Dichlorobenzene-d4	11.819

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dodecane	170	C12H26	000112-40-3	93
2		Tetradecane	198	C14H30	000629-59-4	64
3		Undecane	156	C11H24	001120-21-4	64
4		Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	59
5		Hexadecane	226	C16H34	000544-76-3	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
Data File : VU045294.D
Acq On : 12 Oct 2021 16:10
Operator : SY/MD
Sample : M4070-09ME
Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E6ME

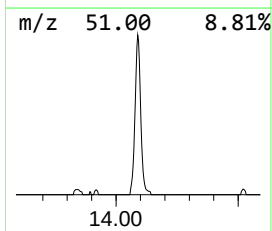
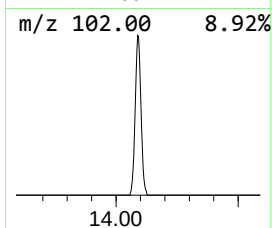
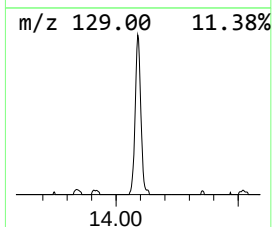
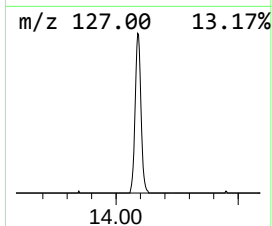
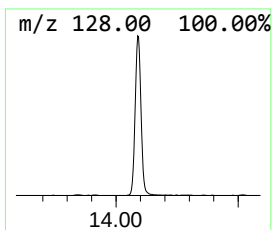
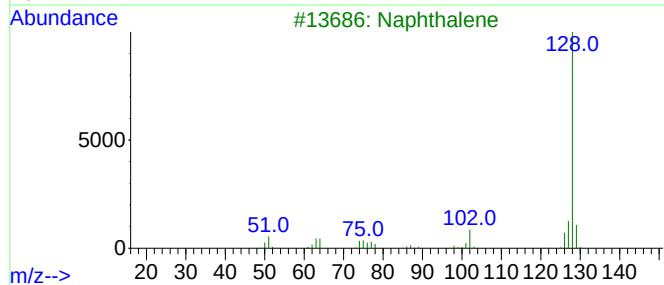
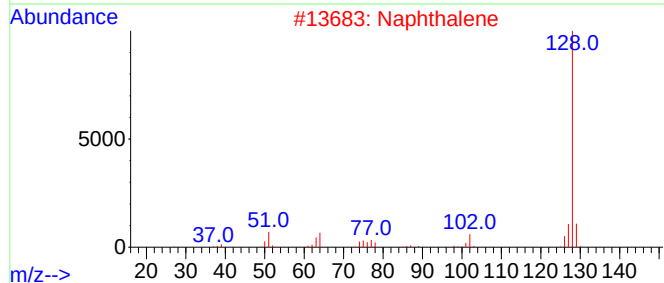
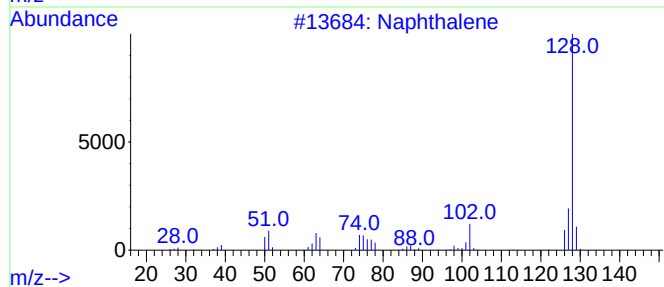
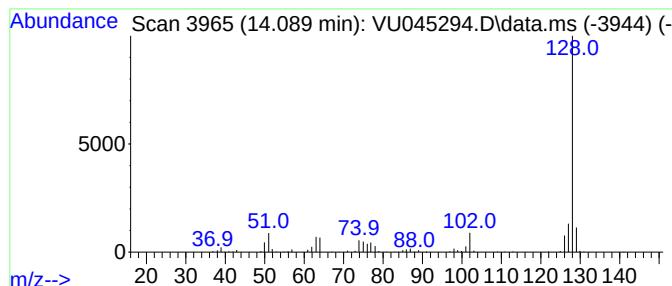
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 16 1H-Indene, 1-methylene- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.089	14.65 ug/L	250228	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	97
2			Naphthalene	128	C10H8	000091-20-3	95
3			Naphthalene	128	C10H8	000091-20-3	95
4			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	95
5			Naphthalene	128	C10H8	000091-20-3	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
Data File : VU045294.D
Acq On : 12 Oct 2021 16:10
Operator : SY/MD
Sample : M4070-09ME
Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E6ME

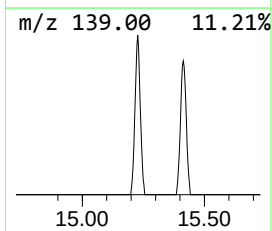
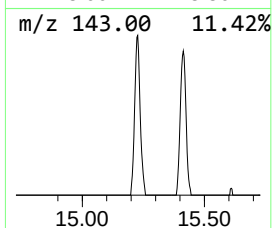
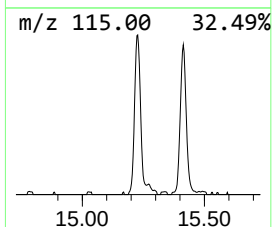
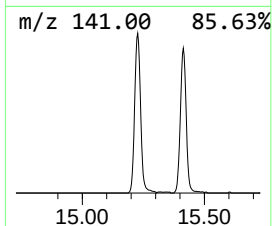
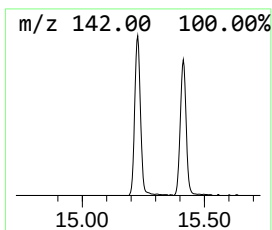
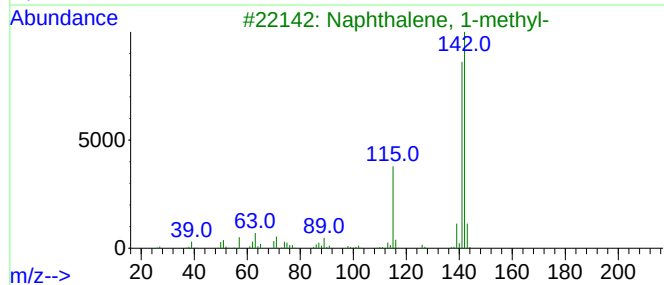
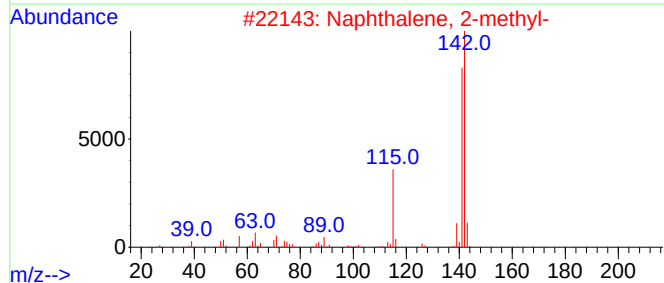
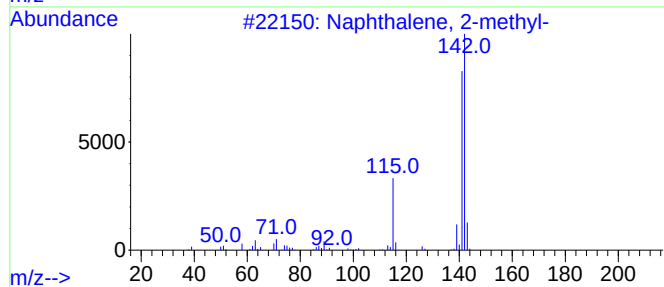
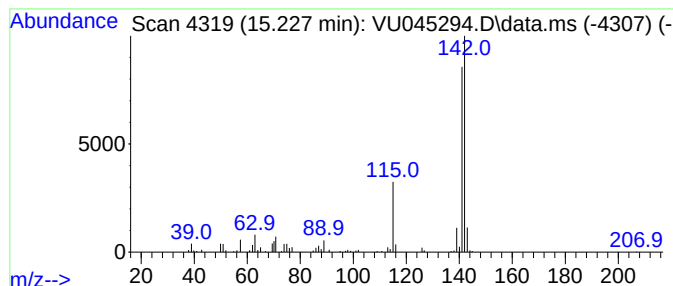
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 17 Naphthalene, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.227	7.80 ug/L	133117	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
4			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
5			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
Data File : VU045294.D
Acq On : 12 Oct 2021 16:10
Operator : SY/MD
Sample : M4070-09ME
Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E6ME

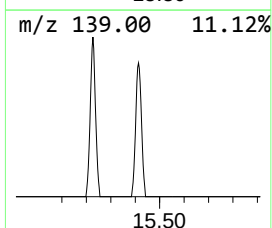
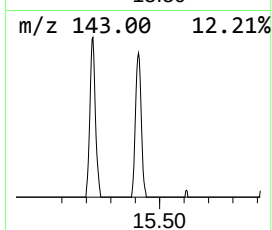
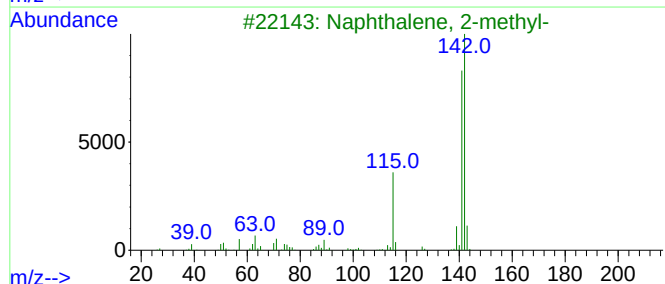
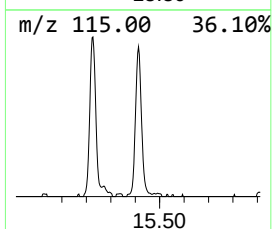
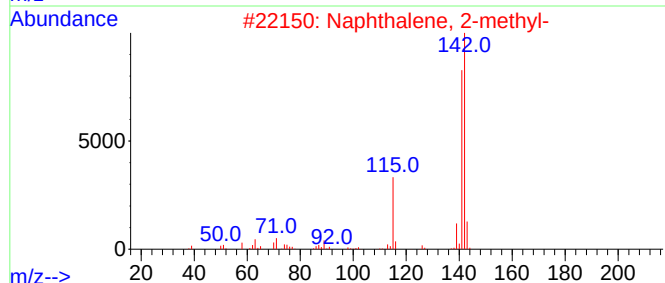
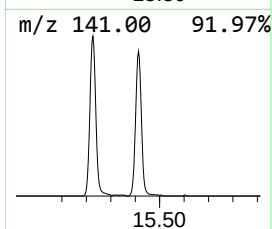
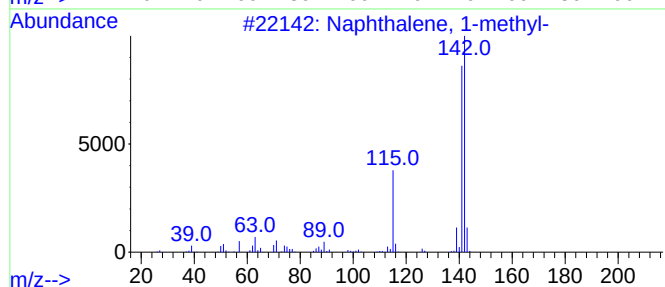
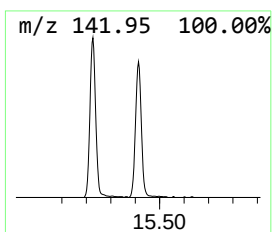
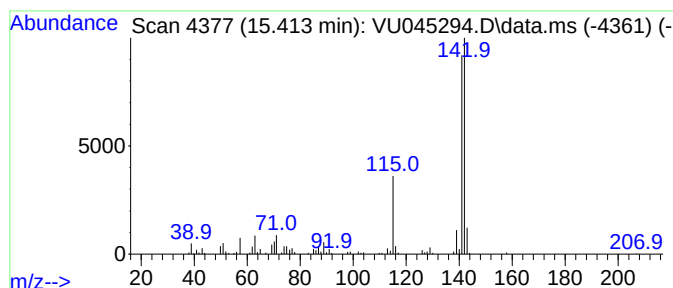
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 18 Naphthalene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.413	7.68 ug/L	131226	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
4			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94
5			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101221\
 Data File : VU045294.D
 Acq On : 12 Oct 2021 16:10
 Operator : SY/MD
 Sample : M4070-09ME
 Misc : 2.53g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW7E6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
 Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.459	3.2	ug/L	43898	1	6.250	693816	50.0
(DEL) Alkane: S...	3.324	3.6	ug/L	50067	1	6.250	693816	50.0
(DEL) Alkane: C...	4.510	8.8	ug/L	122021	1	6.250	693816	50.0
(DEL) Alkane: C...	5.841	4.1	ug/L	56986	1	6.250	693816	50.0
(DEL) Alkane: C...	5.912	3.4	ug/L	47586	1	6.250	693816	50.0
(DEL) Alkane: C...	5.980	7.6	ug/L	105424	1	6.250	693816	50.0
(DEL) Alkane: C...	7.070	2.5	ug/L	35275	1	6.250	693816	50.0
(DEL) Alkane: C...	7.230	2.8	ug/L	38230	1	6.250	693816	50.0
(DEL) Alkane: C...	8.864	2.7	ug/L	47437	2	9.426	865066	50.0
Benzene, propyl-	10.912	5.4	ug/L	91911	3	11.819	853788	50.0
Benzene, 1-ethy...	11.005	5.6	ug/L	95206	3	11.819	853788	50.0
Benzene, 1-ethy...	11.298	3.5	ug/L	59442	3	11.819	853788	50.0
Benzene, 1,2,3-...	11.899	3.9	ug/L	66592	3	11.819	853788	50.0
(DEL) Alkane: S...	13.436	3.4	ug/L	57205	3	11.819	853788	50.0
1H-Indene, 1-me...	14.089	14.7	ug/L	250228	3	11.819	853788	50.0
Naphthalene, 2-...	15.227	7.8	ug/L	133117	3	11.819	853788	50.0
Naphthalene, 1-...	15.413	7.7	ug/L	131226	3	11.819	853788	50.0