

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
 Data File : VU045253.D
 Acq On : 08 Oct 2021 15:53
 Operator : SY/MD
 Sample : M4070-07ME
 Misc : 2.54g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW7E0ME

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: VU045253.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.456	29	36	52	rBV	156413	240246	5.96%	1.311%
2	1.597	73	80	101	rVB	107826	137292	3.41%	0.749%
3	1.871	159	165	177	rBV	47543	57241	1.42%	0.312%
4	2.523	355	368	387	rBV	200856	349224	8.67%	1.906%
5	2.607	388	394	426	rVB2	7969	22129	0.55%	0.121%
6	2.758	431	441	446	rVB2	669	1023	0.03%	0.006%
7	2.970	496	507	511	rBV2	891	1637	0.04%	0.009%
8	3.035	517	527	542	rVB4	12548	28818	0.72%	0.157%
9	3.173	562	570	573	rBV3	403	562	0.01%	0.003%
10	3.324	604	617	630	rVB5	3062	6994	0.17%	0.038%
11	3.494	666	670	674	rBV	233	266	0.01%	0.001%
12	3.620	705	709	715	rVB2	236	277	0.01%	0.002%
13	3.671	715	725	735	rVB4	2350	4791	0.12%	0.026%
14	3.861	771	784	796	rBV2	1397	3310	0.08%	0.018%
15	4.285	912	916	920	rVB2	202	223	0.01%	0.001%
16	4.391	942	949	952	rBV2	229	275	0.01%	0.002%
17	4.510	973	986	999	rBV3	6484	14740	0.37%	0.080%
18	4.645	1004	1028	1043	rBV	113832	328953	8.17%	1.795%
19	5.063	1141	1158	1179	rVV	211051	485723	12.06%	2.650%
20	5.311	1220	1235	1244	rBV4	9758	21282	0.53%	0.116%
21	5.449	1269	1278	1291	rVB3	1790	3070	0.08%	0.017%
22	5.581	1309	1319	1328	rVV3	2702	4834	0.12%	0.026%
23	5.719	1340	1362	1390	rVV2	497681	1270092	31.53%	6.931%
24	5.842	1390	1400	1411	rVV5	3563	7174	0.18%	0.039%
25	5.916	1412	1423	1433	rVV7	2215	4499	0.11%	0.025%
26	5.980	1433	1443	1460	rVB5	8518	18016	0.45%	0.098%
27	6.125	1479	1488	1498	rVB5	3569	6315	0.16%	0.034%
28	6.250	1511	1527	1552	rVV	359107	702993	17.45%	3.836%
29	6.533	1605	1615	1624	rBV7	4412	8562	0.21%	0.047%
30	6.604	1629	1637	1650	rVB5	3651	7881	0.20%	0.043%
31	6.694	1650	1665	1678	rBV	291042	586937	14.57%	3.203%
32	6.861	1715	1717	1725	rVV3	475	406	0.01%	0.002%
33	6.980	1746	1754	1759	rBV2	1830	2576	0.06%	0.014%
34	7.067	1768	1781	1790	rBV5	1990	4239	0.11%	0.023%
35	7.189	1810	1819	1825	rBV2	3424	5626	0.14%	0.031%
36	7.427	1886	1893	1900	rBV4	1172	1706	0.04%	0.009%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Peak Location: TOP

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

37	7.497	1903	1915	1922	rBV3	6972	12079	0.30%	0.066%
38	7.568	1924	1937	1957	rVB	149120	276899	6.87%	1.511%
39	7.658	1957	1965	1973	rBV5	4893	8040	0.20%	0.044%
40	7.816	2001	2014	2021	rBV2	27738	62215	1.54%	0.339%
41	7.903	2029	2041	2052	rVV	547076	963862	23.93%	5.259%
42	7.973	2052	2063	2088	rVB	246050	443382	11.01%	2.419%
43	8.057	2088	2089	2091	rBV	708	376	0.01%	0.002%
44	8.131	2105	2112	2119	rVB2	9849	12626	0.31%	0.069%
45	8.186	2119	2129	2141	rBV	98109	179199	4.45%	0.978%
46	8.369	2175	2186	2197	rVB4	8442	14885	0.37%	0.081%
47	8.430	2201	2205	2207	rBV2	446	352	0.01%	0.002%
48	8.475	2212	2219	2225	rVB5	1279	2009	0.05%	0.011%
49	8.552	2230	2243	2254	rVB5	11174	19901	0.49%	0.109%
50	8.649	2258	2273	2301	rBV	417769	785442	19.50%	4.286%
51	8.803	2315	2321	2330	rBV7	6388	10920	0.27%	0.060%
52	8.864	2334	2340	2350	rVB4	21138	35522	0.88%	0.194%
53	8.925	2351	2359	2368	rBV2	9513	14629	0.36%	0.080%
54	9.066	2397	2403	2404	rBV2	2198	1580	0.04%	0.009%
55	9.124	2412	2421	2426	rBV3	5219	8453	0.21%	0.046%
56	9.166	2427	2434	2442	rVV5	10959	19824	0.49%	0.108%
57	9.214	2443	2449	2459	rVB3	13127	20882	0.52%	0.114%
58	9.337	2475	2487	2500	rBV3	10541	17383	0.43%	0.095%
59	9.423	2500	2514	2535	rBV	512440	901442	22.38%	4.919%
60	9.510	2536	2541	2548	rVB5	1978	2924	0.07%	0.016%
61	9.575	2548	2561	2575	rBV	526394	893452	22.18%	4.875%
62	9.697	2585	2599	2633	rVB	2351993	4028362	100.00%	21.982%
63	9.841	2639	2644	2647	rBV3	274	333	0.01%	0.002%
64	9.883	2651	2657	2661	rBV3	701	893	0.02%	0.005%
65	9.951	2674	2678	2681	rBV3	642	481	0.01%	0.003%
66	10.031	2690	2703	2704	rBV5	5758	8020	0.20%	0.044%
67	10.108	2713	2727	2744	rVB	745986	1213498	30.12%	6.622%
68	10.253	2756	2772	2786	rBV7	8968	22877	0.57%	0.125%
69	10.320	2788	2793	2796	rBV5	921	1046	0.03%	0.006%
70	10.356	2797	2804	2811	rBV7	5621	9666	0.24%	0.053%
71	10.491	2830	2846	2855	rBV2	10313	20692	0.51%	0.113%
72	10.558	2855	2867	2877	rBV7	4785	10716	0.27%	0.058%
73	10.764	2919	2931	2943	rBV	472337	741027	18.40%	4.044%
74	10.912	2968	2977	2985	rBV2	14716	22166	0.55%	0.121%
75	11.005	2996	3006	3020	rBV	55288	112663	2.80%	0.615%
76	11.095	3026	3034	3056	rVB2	72451	177000	4.39%	0.966%

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Integration Parameters: LSCINT.P

Integrator: RTE

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 Title : VOC Analysis

77	11.240	3073	3079	3086	rVB3	5727	7999	0.20%	0.044%
78	11.298	3088	3097	3113	rVV	32560	60895	1.51%	0.332%
79	11.378	3117	3122	3126	rVV7	5662	7883	0.20%	0.043%
80	11.420	3128	3135	3141	rVV2	32660	48444	1.20%	0.264%
81	11.472	3142	3151	3172	rVB	141445	242473	6.02%	1.323%
82	11.816	3247	3258	3271	rBV	562417	897070	22.27%	4.895%
83	11.902	3273	3285	3298	rVB3	46579	104292	2.59%	0.569%
84	12.198	3365	3377	3390	rBV	617806	1007705	25.02%	5.499%
85	12.330	3410	3418	3428	rVB	123436	170147	4.22%	0.928%
86	12.475	3456	3463	3466	rBV2	15767	22302	0.55%	0.122%
87	12.671	3517	3524	3530	rBV2	20002	28942	0.72%	0.158%
88	13.356	3732	3737	3746	rBV9	8013	11168	0.28%	0.061%
89	13.436	3755	3762	3783	rVB4	73970	174213	4.32%	0.951%
90	13.838	3881	3887	3893	rBV6	6657	10284	0.26%	0.056%
91	14.089	3960	3965	3986	rVB	26893	53444	1.33%	0.292%
92	14.188	3987	3996	4009	rVV7	6402	13055	0.32%	0.071%
93	14.452	4071	4078	4087	rVB3	12088	16157	0.40%	0.088%
94	14.777	4176	4179	4182	rBV4	715	541	0.01%	0.003%
95	14.934	4225	4228	4232	rBV3	538	601	0.01%	0.003%
96	15.021	4252	4255	4256	rBV2	479	284	0.01%	0.002%
97	15.063	4263	4268	4269	rBV3	855	707	0.02%	0.004%
98	15.143	4290	4293	4295	rBV2	451	289	0.01%	0.002%
99	15.227	4309	4319	4332	rBV3	9217	15348	0.38%	0.084%
100	15.414	4367	4377	4391	rBV4	7954	14222	0.35%	0.078%

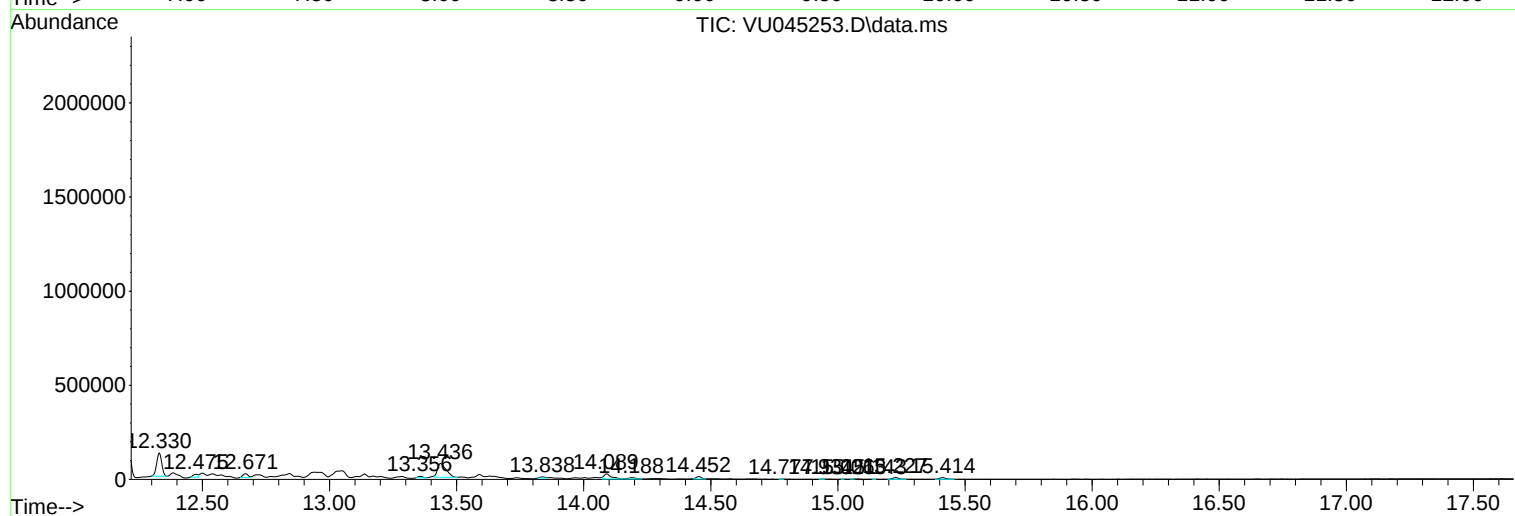
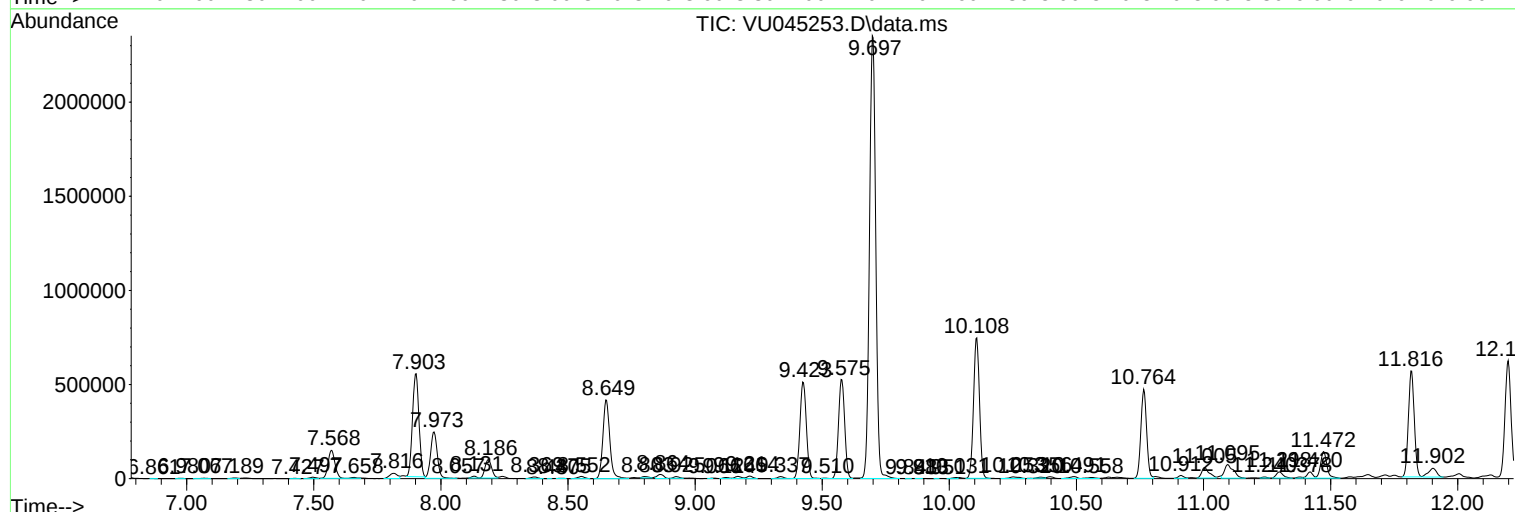
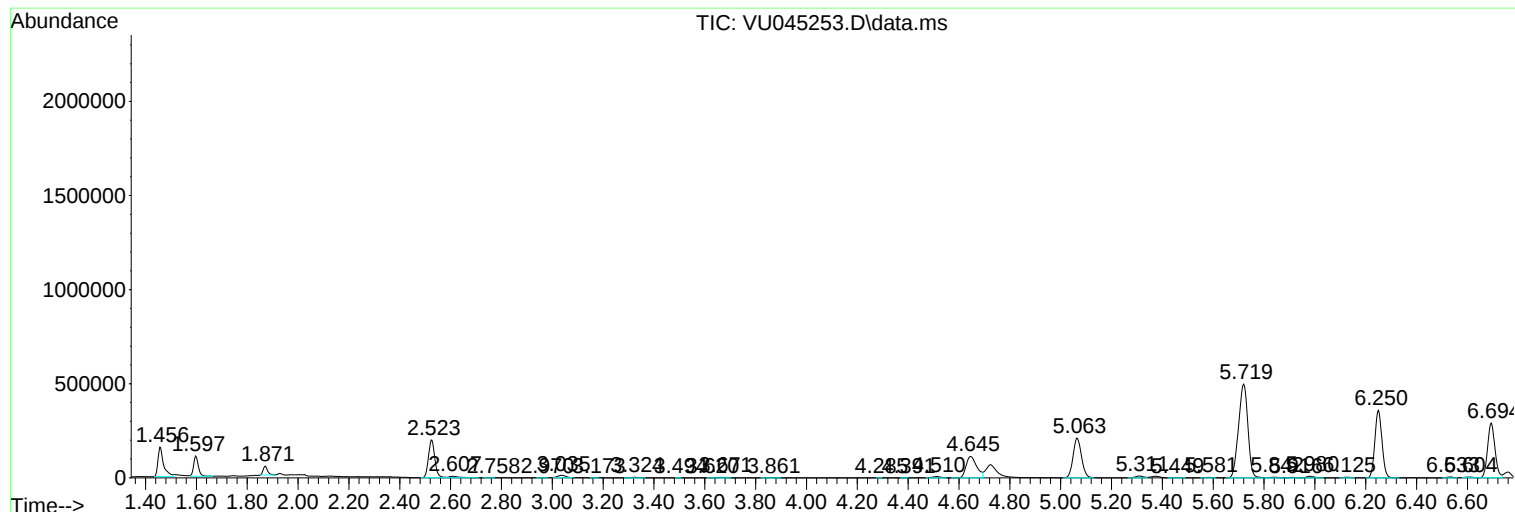
Sum of corrected areas: 18326115

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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E0ME

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



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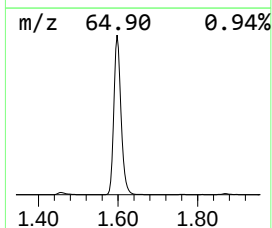
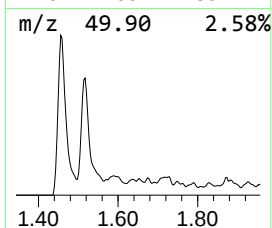
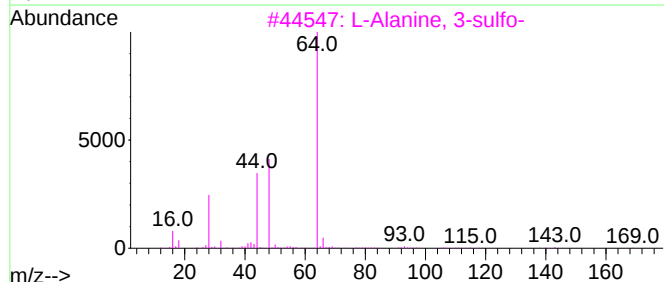
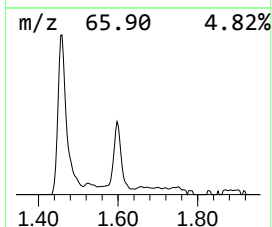
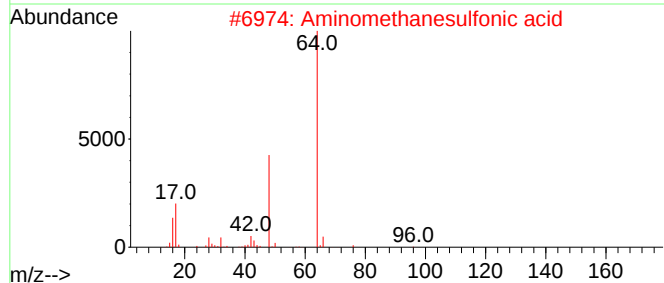
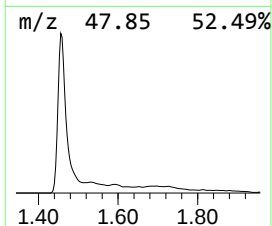
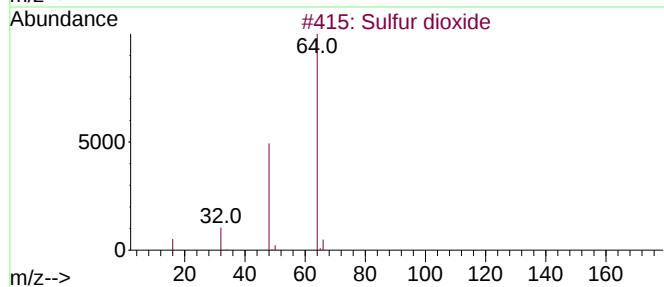
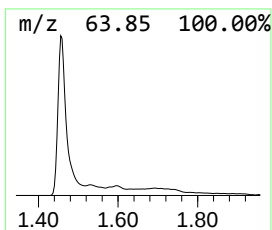
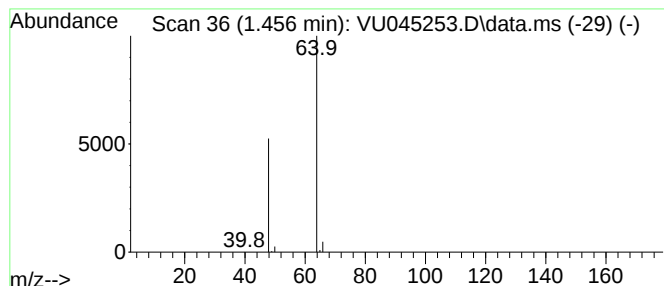
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.456	17.09 ug/L	240246	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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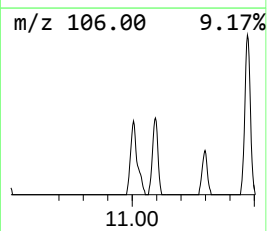
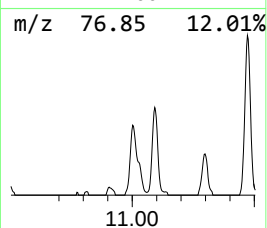
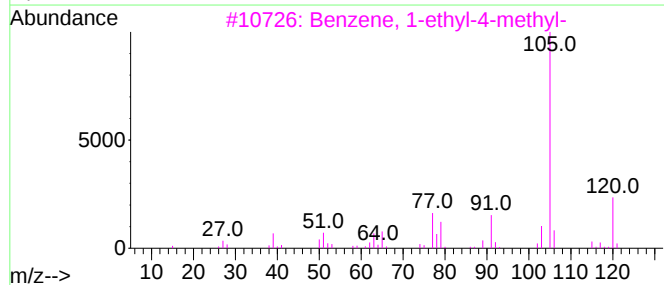
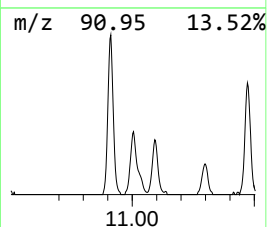
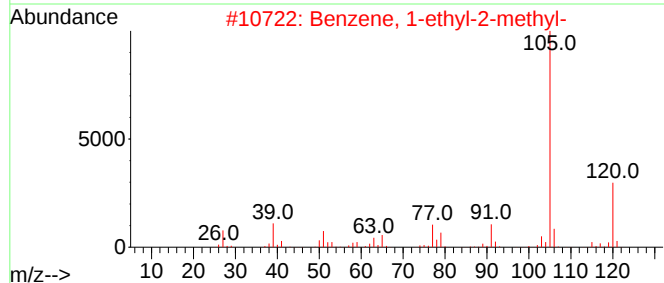
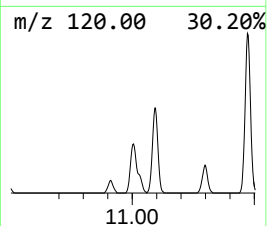
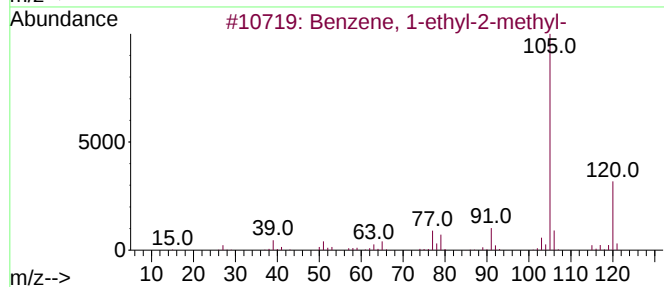
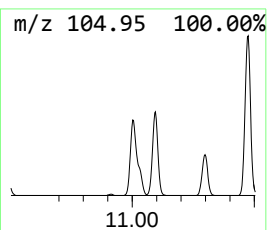
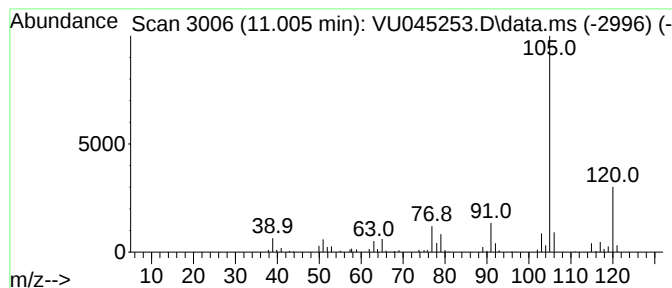
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Benzene, 1-ethyl-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.005	6.28 ug/L	112663	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-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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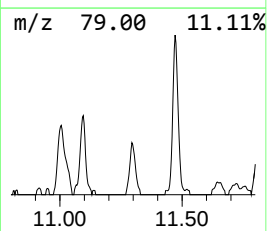
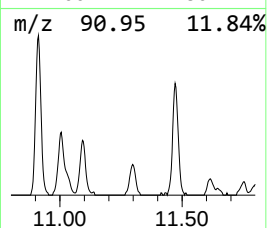
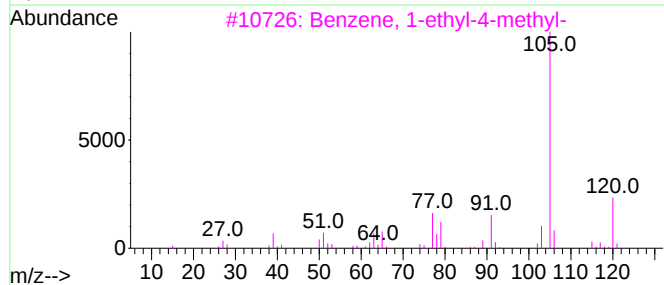
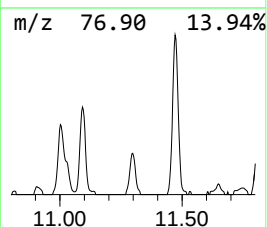
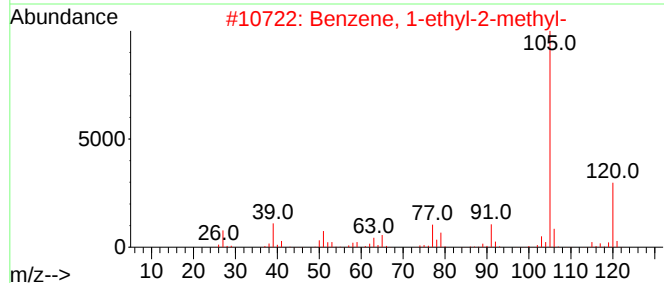
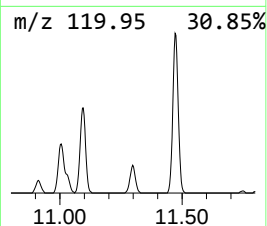
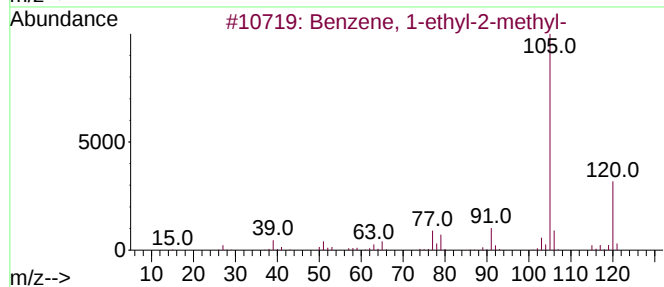
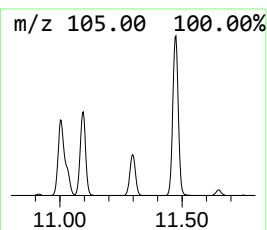
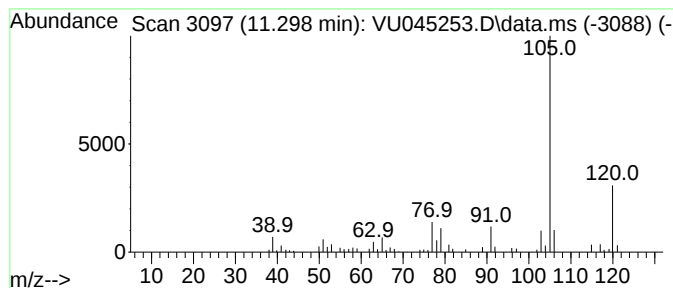
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Quant Title : VOC Analysis

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

Peak Number 4 Benzene, 1-ethyl-4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.298	3.39 ug/L	60895	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	94
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	94
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
Data File : VU045253.D
Acq On : 08 Oct 2021 15:53
Operator : SY/MD
Sample : M4070-07ME
Misc : 2.54g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E0ME

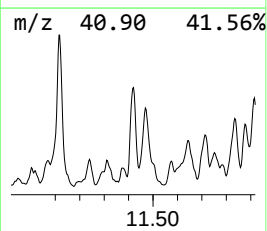
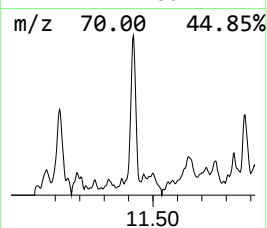
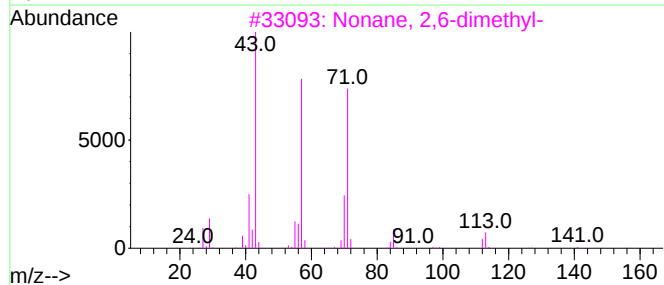
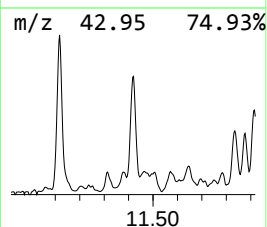
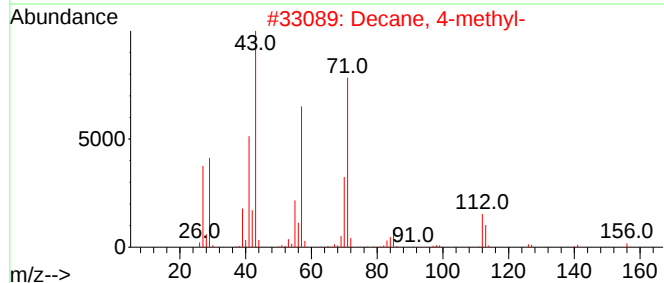
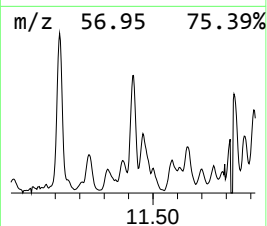
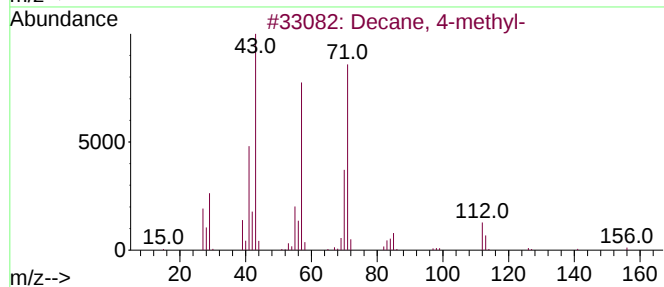
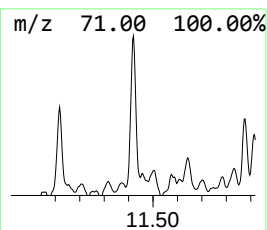
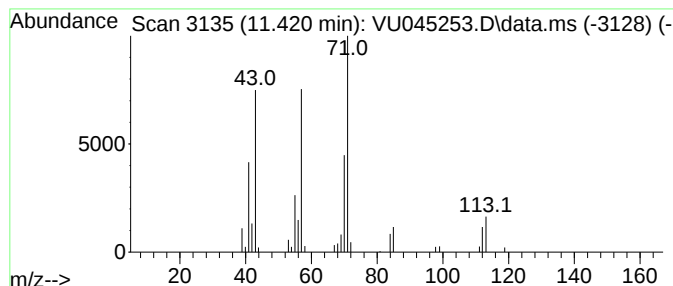
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Quant Title : VOC Analysis

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

Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.420	2.70 ug/L	48444	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 4-methyl-	156	C11H24	002847-72-5	83
2			Decane, 4-methyl-	156	C11H24	002847-72-5	83
3			Nonane, 2,6-dimethyl-	156	C11H24	017302-28-2	78
4			Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	72
5			Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	64



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
Data File : VU045253.D
Acq On : 08 Oct 2021 15:53
Operator : SY/MD
Sample : M4070-07ME
Misc : 2.54g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E0ME

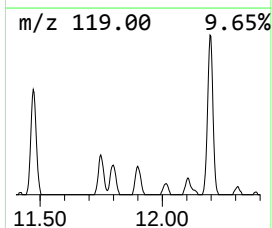
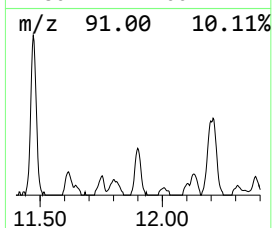
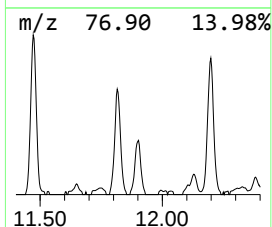
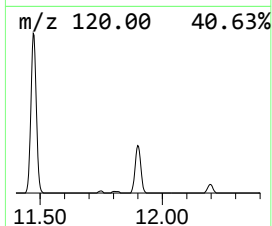
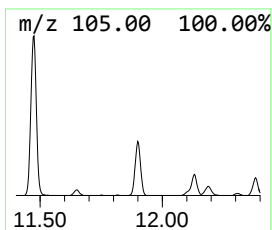
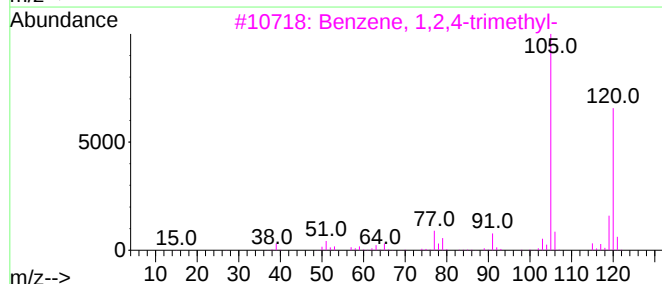
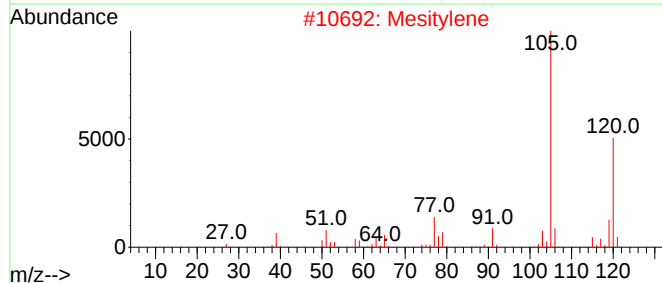
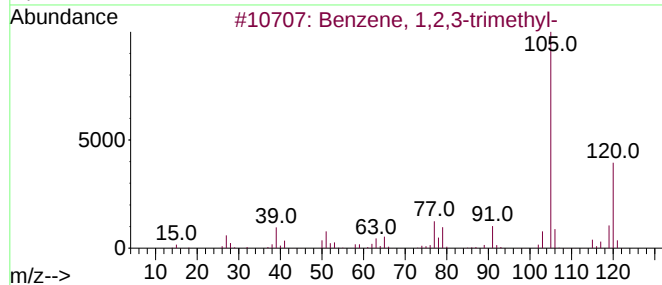
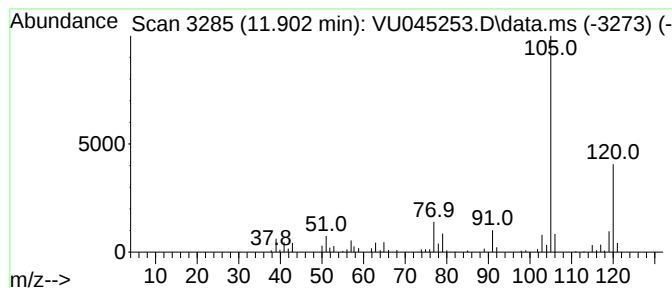
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Quant Title : VOC Analysis

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

Peak Number 6 Benzene, 1,2,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.902	5.81 ug/L	104292	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	97
2			Mesitylene	120	C9H12	000108-67-8	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
Data File : VU045253.D
Acq On : 08 Oct 2021 15:53
Operator : SY/MD
Sample : M4070-07ME
Misc : 2.54g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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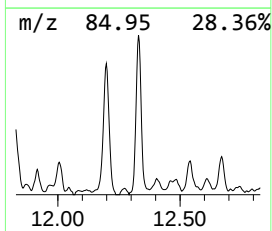
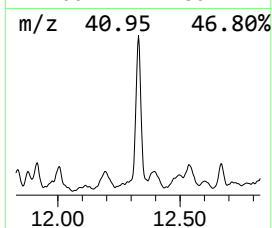
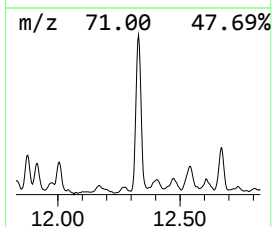
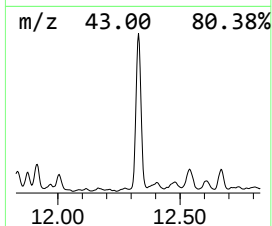
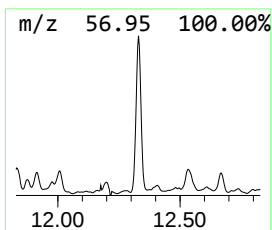
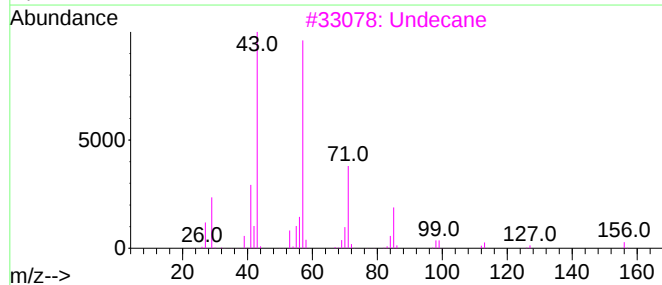
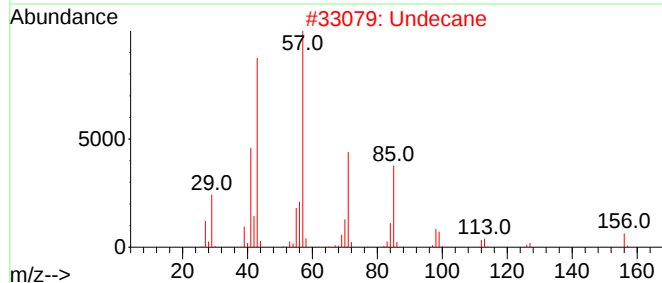
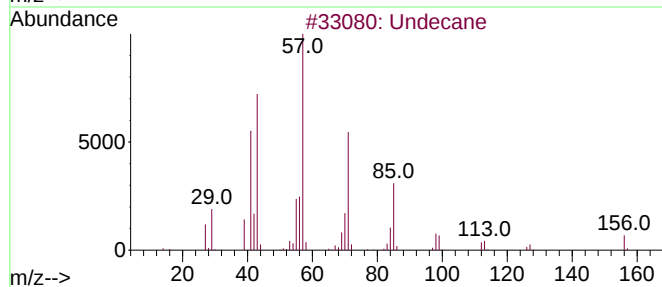
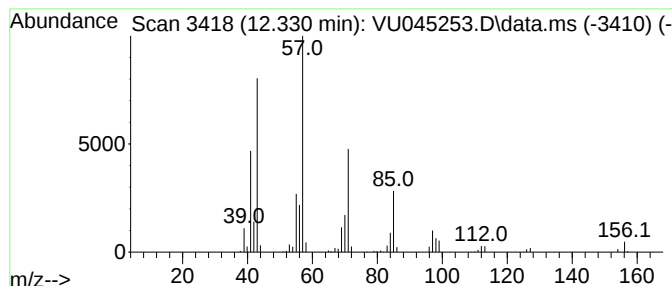
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Quant Title : VOC Analysis

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

Peak Number 7 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.330	9.48 ug/L	170147	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecane			156	C11H24	001120-21-4	93
2	Undecane			156	C11H24	001120-21-4	93
3	Undecane			156	C11H24	001120-21-4	90
4	Carbonic acid, prop-1-en-2-yl tr...			284	C17H32O3	1000382-90-8	90
5	Decane			142	C10H22	000124-18-5	86



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
Data File : VU045253.D
Acq On : 08 Oct 2021 15:53
Operator : SY/MD
Sample : M4070-07ME
Misc : 2.54g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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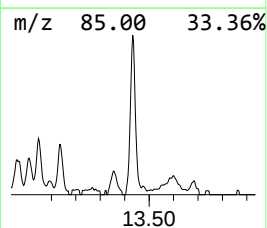
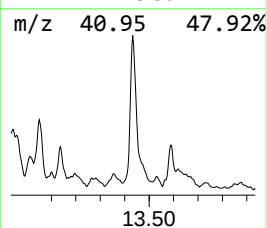
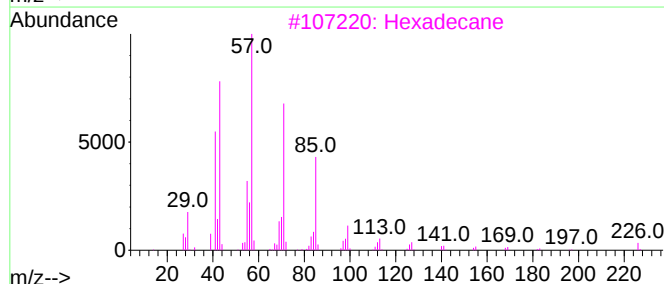
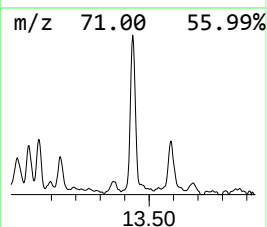
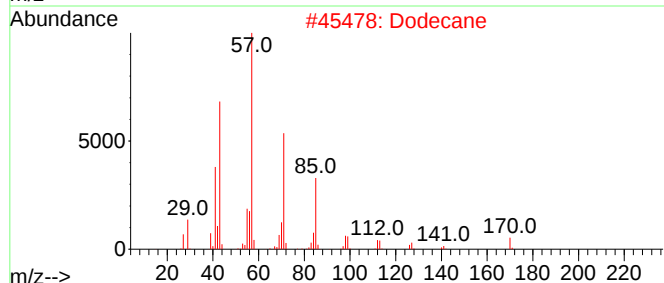
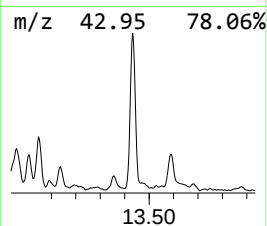
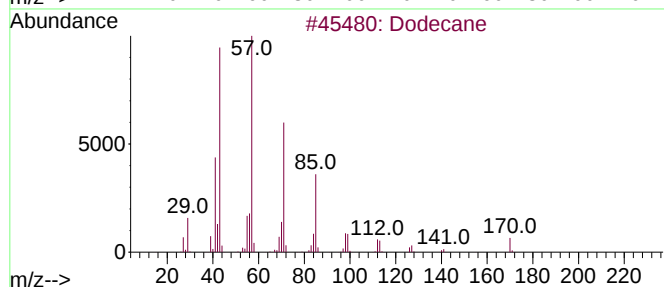
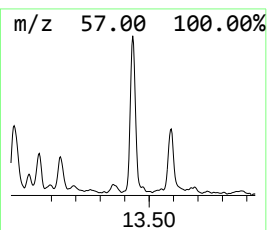
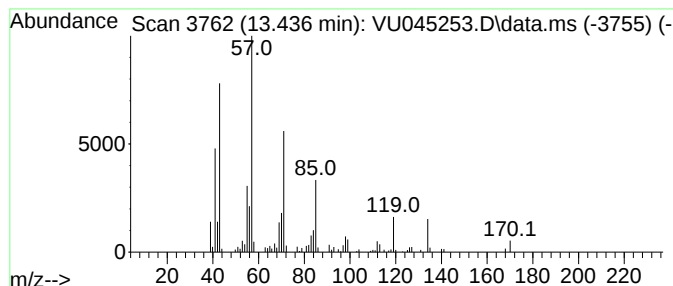
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Quant Title : VOC Analysis

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

Peak Number 8 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.436	9.71 ug/L	174213	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane	170	C12H26	000112-40-3	94
2			Dodecane	170	C12H26	000112-40-3	93
3			Hexadecane	226	C16H34	000544-76-3	72
4			Undecane	156	C11H24	001120-21-4	72
5			Dodecane	170	C12H26	000112-40-3	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
Data File : VU045253.D
Acq On : 08 Oct 2021 15:53
Operator : SY/MD
Sample : M4070-07ME
Misc : 2.54g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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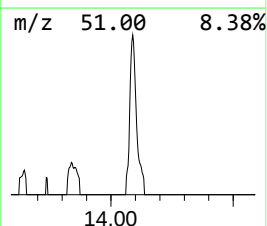
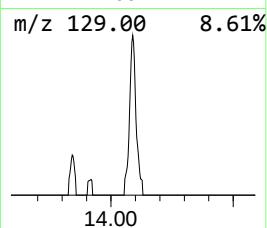
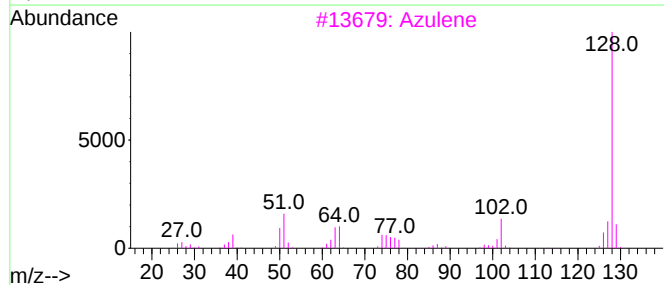
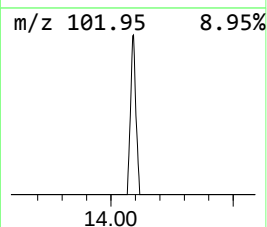
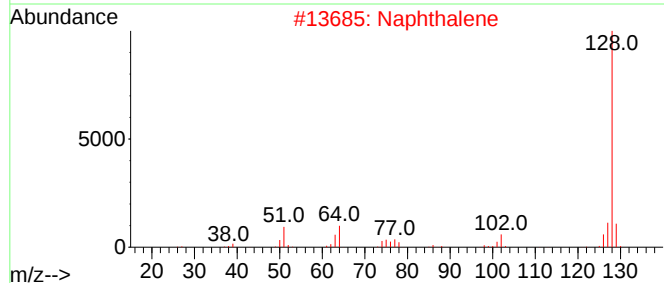
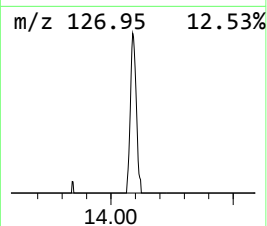
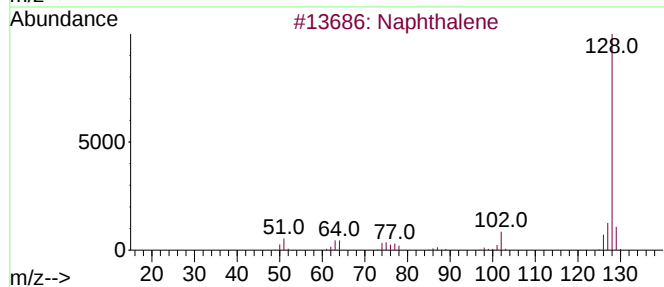
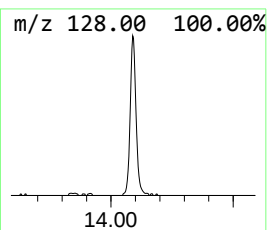
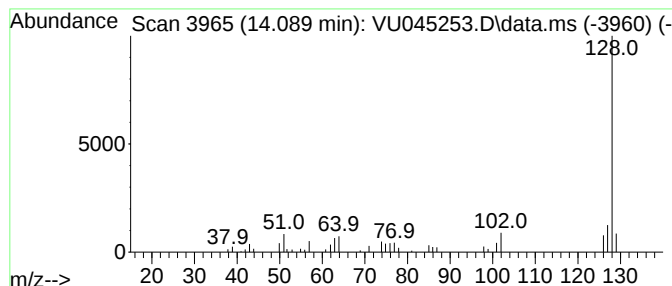
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Quant Title : VOC Analysis

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

Peak Number 9 Azulene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.089	2.98 ug/L	53444	1,4-Dichlorobenzene-d4	11.819

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	91
2			Naphthalene	128	C10H8	000091-20-3	91
3			Azulene	128	C10H8	000275-51-4	91
4			Azulene	128	C10H8	000275-51-4	91
5			Naphthalene	128	C10H8	000091-20-3	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100821\
Data File : VU045253.D
Acq On : 08 Oct 2021 15:53
Operator : SY/MD
Sample : M4070-07ME
Misc : 2.54g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW7E0ME

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	1.456	17.1	ug/L	240246	1	6.250	702993	50.0
Benzene, 1-ethy...	11.005	6.3	ug/L	112663	3	11.819	897070	50.0
Benzene, 1-ethy...	11.298	3.4	ug/L	60895	3	11.819	897070	50.0
(DEL) Alkane: S...	11.420	2.7	ug/L	48444	3	11.819	897070	50.0
Benzene, 1,2,3-...	11.902	5.8	ug/L	104292	3	11.819	897070	50.0
(DEL) Alkane: S...	12.330	9.5	ug/L	170147	3	11.819	897070	50.0
(DEL) Alkane: S...	13.436	9.7	ug/L	174213	3	11.819	897070	50.0
Azulene	14.089	3.0	ug/L	53444	3	11.819	897070	50.0