

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100521\
 Data File : VU045138.D
 Acq On : 05 Oct 2021 12:37
 Operator : SY/MD
 Sample : M3974-09ME
 Misc : 5.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW8Z3ME

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: VU045138.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	39	44	51	rBV2	7810	11248	0.49%	0.080%
2	1.600	73	81	98	rVB	130044	198543	8.64%	1.415%
3	1.899	167	174	191	rBV	52852	91043	3.96%	0.649%
4	2.536	358	372	390	rBV	253626	458746	19.97%	3.269%
5	2.961	495	504	507	rBV2	460	758	0.03%	0.005%
6	3.044	517	530	546	rVV6	4095	10678	0.46%	0.076%
7	3.112	546	551	559	rVB4	505	620	0.03%	0.004%
8	3.179	565	572	579	rBV4	942	1790	0.08%	0.013%
9	3.330	612	619	629	rVV4	1536	2561	0.11%	0.018%
10	3.674	718	726	739	rVB5	2106	3960	0.17%	0.028%
11	4.520	977	989	999	rBV5	2708	6259	0.27%	0.045%
12	4.661	1013	1033	1085	rBV2	205874	692583	30.16%	4.935%
13	5.067	1140	1159	1185	rBV	220301	533950	23.25%	3.805%
14	5.202	1199	1201	1211	rVB4	414	307	0.01%	0.002%
15	5.285	1220	1227	1228	rBV3	604	528	0.02%	0.004%
16	5.378	1244	1256	1268	rVB6	3475	7648	0.33%	0.054%
17	5.587	1315	1321	1328	rVB4	824	1015	0.04%	0.007%
18	5.632	1333	1335	1342	rVB3	428	303	0.01%	0.002%
19	5.722	1342	1363	1392	rBV2	547210	1408366	61.32%	10.036%
20	5.906	1417	1420	1432	rVB4	1164	1685	0.07%	0.012%
21	5.986	1432	1445	1471	rBV3	10934	27227	1.19%	0.194%
22	6.124	1479	1488	1496	rVB6	1147	1828	0.08%	0.013%
23	6.250	1511	1527	1556	rBV	369362	770471	33.55%	5.490%
24	6.542	1592	1618	1650	rBV	1170590	2296677	100.00%	16.366%
25	6.694	1651	1665	1693	rBV	300553	642801	27.99%	4.580%
26	6.980	1748	1754	1762	rVB4	960	1217	0.05%	0.009%
27	7.060	1772	1779	1781	rBV2	282	350	0.02%	0.002%
28	7.192	1809	1820	1821	rBV2	2010	2053	0.09%	0.015%
29	7.401	1877	1885	1893	rBV3	333	570	0.02%	0.004%
30	7.443	1893	1898	1899	rBV2	531	465	0.02%	0.003%
31	7.571	1921	1938	1964	rBV	160215	324602	14.13%	2.313%
32	7.687	1969	1974	1975	rBV2	801	583	0.03%	0.004%
33	7.758	1990	1996	2003	rVB4	948	1122	0.05%	0.008%
34	7.902	2019	2041	2057	rBV	604701	1129781	49.19%	8.051%
35	7.970	2058	2062	2080	rVB4	8750	15635	0.68%	0.111%
36	8.185	2115	2129	2158	rBV	98090	222144	9.67%	1.583%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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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\SFAMULM092321WMA.M
 Title : VOC Analysis

37	8.362	2177	2184	2185	rBV2	533	483	0.02%	0.003%
38	8.372	2185	2187	2191	rVB	584	341	0.01%	0.002%
39	8.555	2235	2244	2252	rBV5	2919	4554	0.20%	0.032%
40	8.674	2260	2281	2306	rBV	341371	769780	33.52%	5.485%
41	8.806	2319	2322	2326	rVB2	507	453	0.02%	0.003%
42	8.867	2334	2341	2351	rVB5	1951	2872	0.13%	0.020%
43	8.925	2351	2359	2365	rBV4	847	1169	0.05%	0.008%
44	9.427	2500	2515	2533	rBV	456118	956398	41.64%	6.815%
45	9.574	2552	2561	2575	rVB	9766	17634	0.77%	0.126%
46	9.703	2592	2601	2611	rVV7	2467	4866	0.21%	0.035%
47	10.034	2699	2704	2707	rBV4	588	633	0.03%	0.005%
48	10.115	2719	2729	2740	rVB5	2330	4054	0.18%	0.029%
49	10.217	2752	2761	2762	rBV2	214	341	0.01%	0.002%
50	10.234	2762	2766	2767	rBV2	433	305	0.01%	0.002%
51	10.275	2772	2779	2786	rVB4	1239	1783	0.08%	0.013%
52	10.359	2800	2805	2813	rBV3	849	1050	0.05%	0.007%
53	10.398	2813	2817	2824	rVB3	806	784	0.03%	0.006%
54	10.494	2838	2847	2858	rVB2	4464	7478	0.33%	0.053%
55	10.623	2884	2887	2890	rBV2	682	507	0.02%	0.004%
56	10.674	2890	2903	2915	rVB3	6350	11517	0.50%	0.082%
57	10.771	2918	2933	2952	rBV	430359	709075	30.87%	5.053%
58	10.873	2957	2965	2969	rVV5	1704	2923	0.13%	0.021%
59	10.915	2969	2978	2990	rVB	8570	15009	0.65%	0.107%
60	11.005	2999	3006	3010	rBV2	3359	4189	0.18%	0.030%
61	11.095	3025	3034	3049	rBV3	9850	18967	0.83%	0.135%
62	11.211	3064	3070	3076	rVB7	1002	1345	0.06%	0.010%
63	11.298	3084	3097	3112	rBV	30915	52985	2.31%	0.378%
64	11.420	3127	3135	3141	rBV4	2072	3725	0.16%	0.027%
65	11.471	3141	3151	3164	rVB4	12050	23587	1.03%	0.168%
66	11.587	3174	3187	3191	rBV6	1646	2726	0.12%	0.019%
67	11.616	3192	3196	3199	rBV2	856	656	0.03%	0.005%
68	11.648	3199	3206	3215	rVB3	3803	5323	0.23%	0.038%
69	11.700	3215	3222	3231	rBV7	2952	5577	0.24%	0.040%
70	11.751	3231	3238	3247	rVB2	6640	9432	0.41%	0.067%
71	11.822	3247	3260	3279	rBV	556932	887703	38.65%	6.326%
72	12.008	3316	3318	3327	rVB5	3254	3711	0.16%	0.026%
73	12.102	3336	3347	3363	rBV3	33516	61628	2.68%	0.439%
74	12.201	3364	3378	3392	rVB	602585	983335	42.82%	7.007%
75	12.307	3407	3411	3413	rBV2	1627	1453	0.06%	0.010%
76	12.385	3428	3435	3451	rVB6	4808	9845	0.43%	0.070%

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Instrument :
 MSVOA_U
 ClientSampleId :
 EW8Z3ME

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	12.471	3451	3462	3468	rBV2	8233	13514	0.59%	0.096%
78	12.574	3487	3494	3502	rBV2	17361	24691	1.08%	0.176%
79	12.616	3502	3507	3516	rVV3	6621	9402	0.41%	0.067%
80	12.687	3520	3529	3549	rVB3	31356	66306	2.89%	0.472%
81	12.767	3549	3554	3560	rBV5	1213	1225	0.05%	0.009%
82	12.880	3582	3589	3598	rVB3	7759	13065	0.57%	0.093%
83	13.034	3629	3637	3647	rVB3	8147	14909	0.65%	0.106%
84	13.118	3655	3663	3677	rBV3	4570	10480	0.46%	0.075%
85	13.201	3685	3689	3696	rBV3	1820	2345	0.10%	0.017%
86	13.256	3701	3706	3710	rBV3	2220	2546	0.11%	0.018%
87	13.298	3711	3719	3730	rVV	14905	22339	0.97%	0.159%
88	13.455	3750	3768	3783	rBV3	82696	150692	6.56%	1.074%
89	13.629	3816	3822	3837	rVB9	7376	12586	0.55%	0.090%
90	13.735	3848	3855	3862	rBV8	4295	6339	0.28%	0.045%
91	13.790	3862	3872	3880	rBV4	11140	18671	0.81%	0.133%
92	13.844	3881	3889	3899	rVV6	8908	15244	0.66%	0.109%
93	13.918	3905	3912	3913	rBV5	4617	5228	0.23%	0.037%
94	13.944	3916	3920	3935	rVB3	15990	26566	1.16%	0.189%
95	14.211	3990	4003	4012	rVB2	16275	34390	1.50%	0.245%
96	14.487	4085	4089	4095	rBV4	5050	5726	0.25%	0.041%
97	14.819	4183	4192	4196	rBV5	4199	6262	0.27%	0.045%
98	14.880	4204	4211	4221	rVB4	8694	13802	0.60%	0.098%
99	15.021	4248	4255	4268	rBV8	7849	14299	0.62%	0.102%
100	15.413	4368	4377	4399	rVB3	42376	82627	3.60%	0.589%

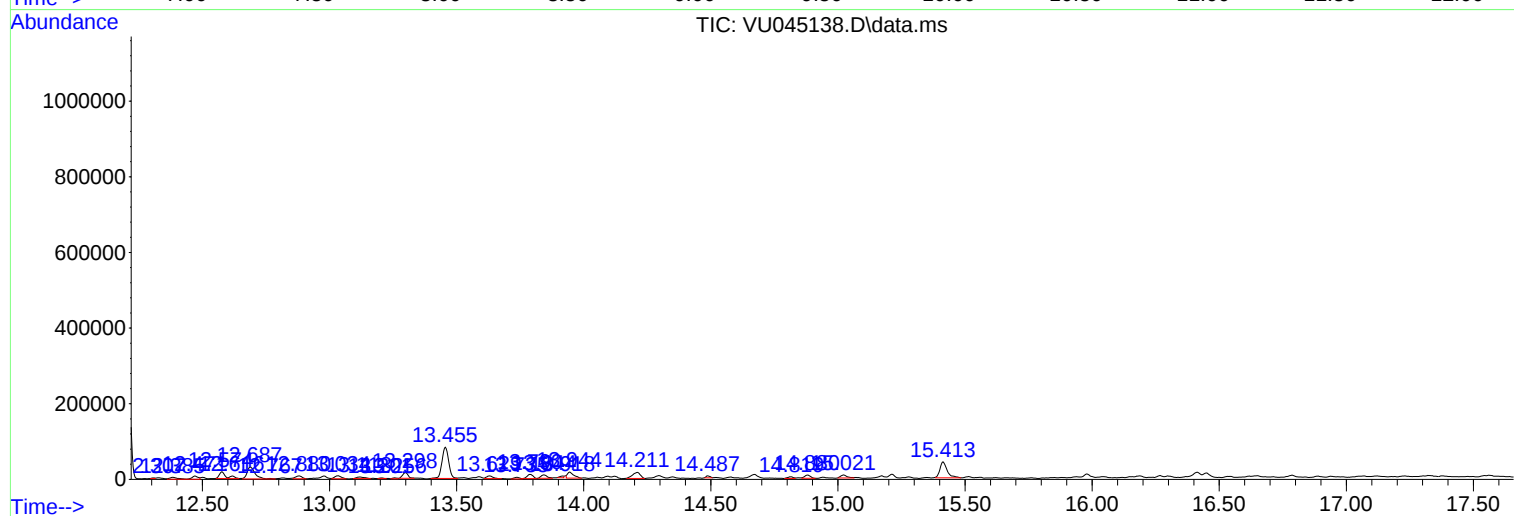
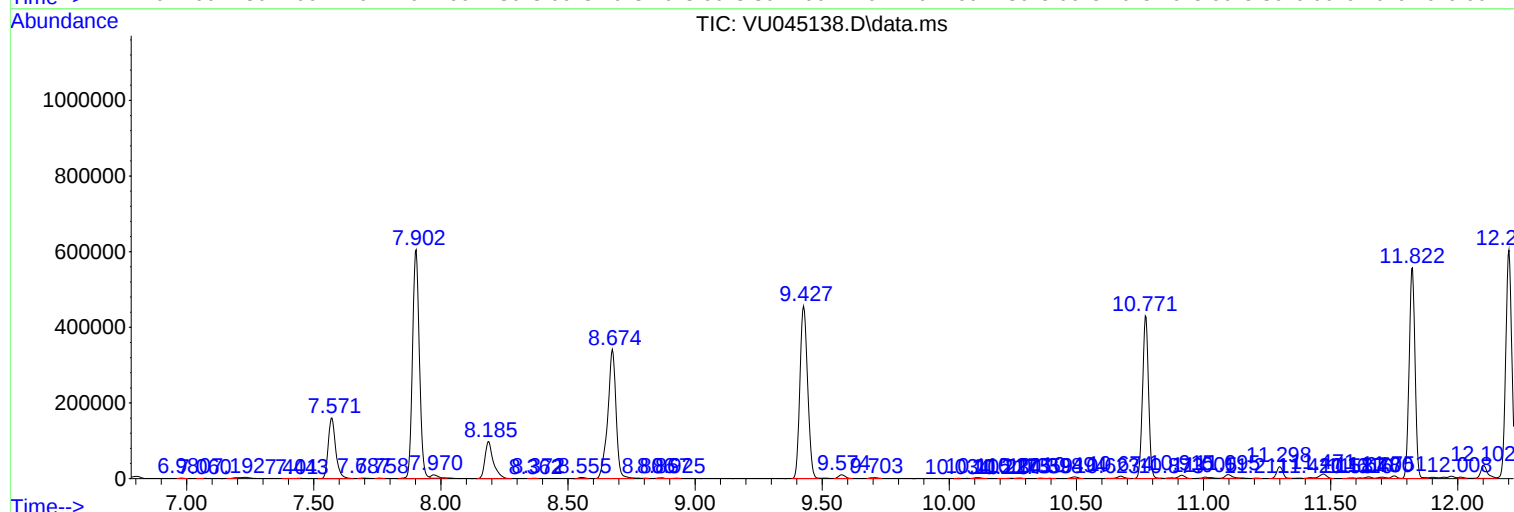
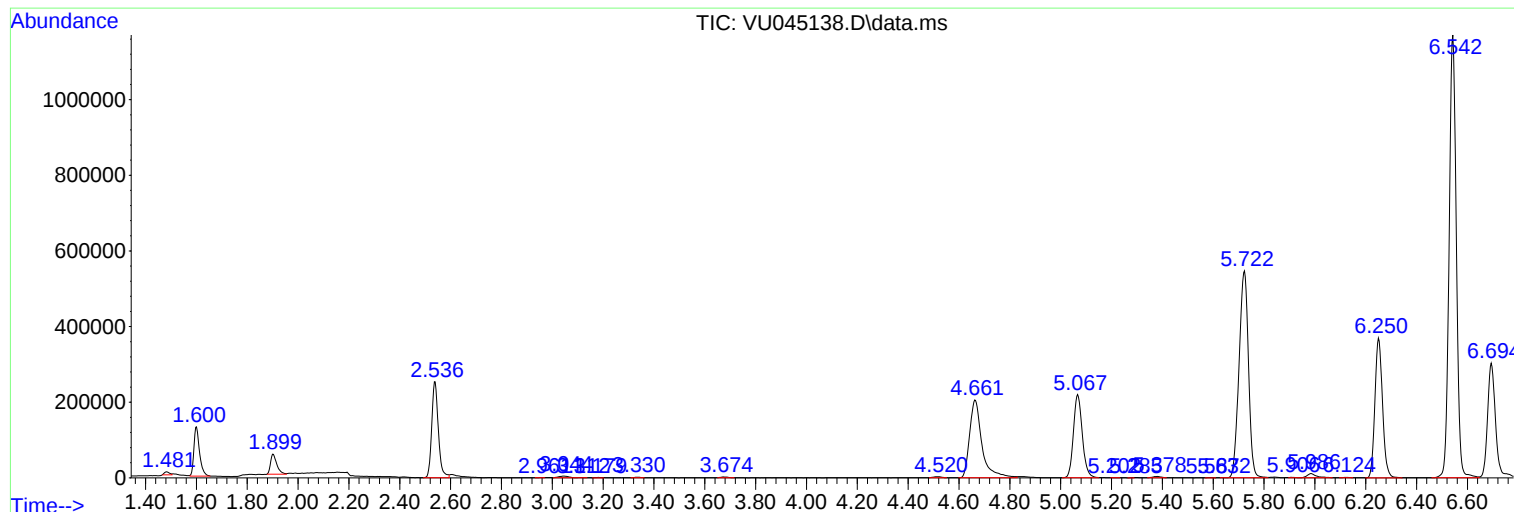
Sum of corrected areas: 14033567

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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW8Z3ME

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\VU100521\
Data File : VU045138.D
Acq On : 05 Oct 2021 12:37
Operator : SY/MD
Sample : M3974-09ME
Misc : 5.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW8Z3ME

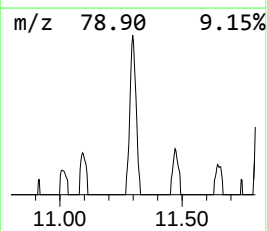
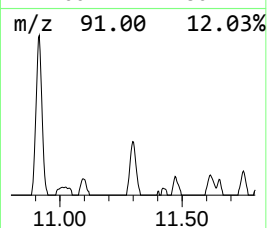
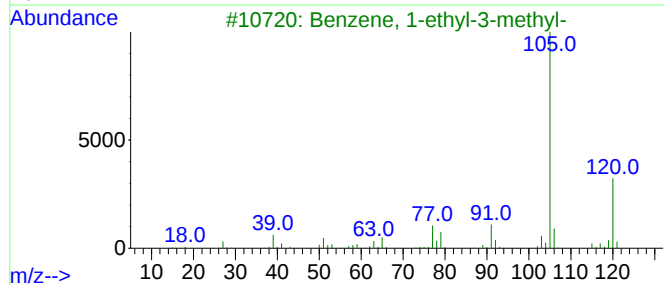
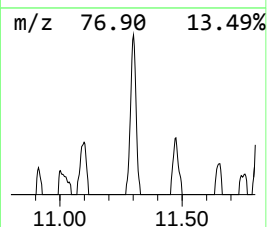
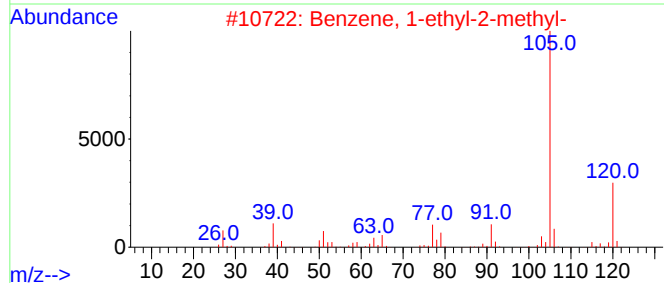
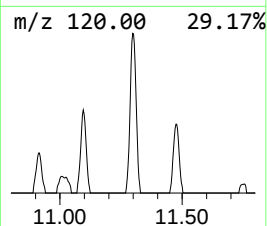
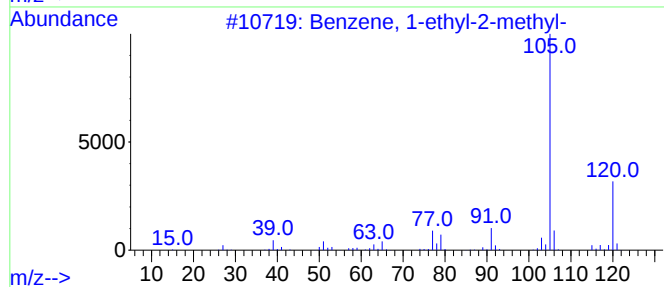
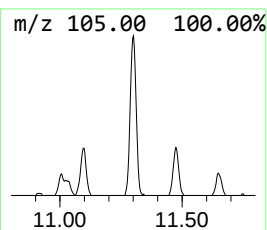
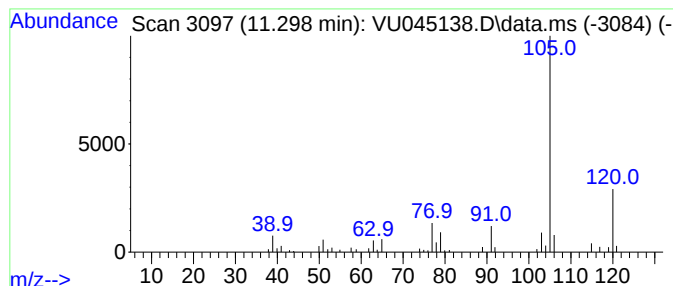
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.298	2.98 ug/L	52985	1,4-Dichlorobenzene-d4	11.822

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	95
3			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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Misc : 5.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW8Z3ME

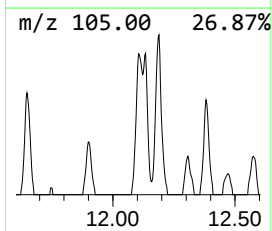
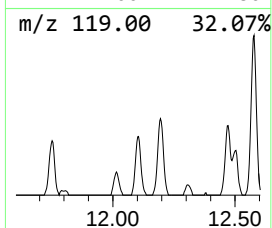
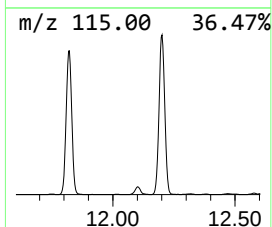
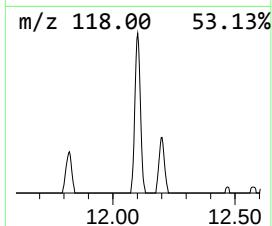
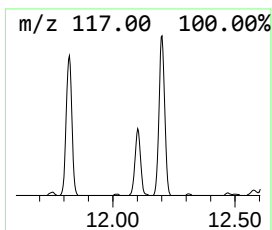
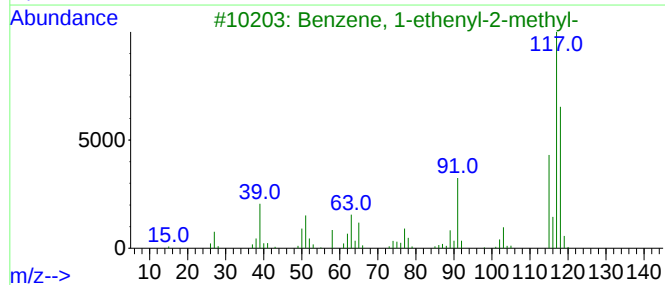
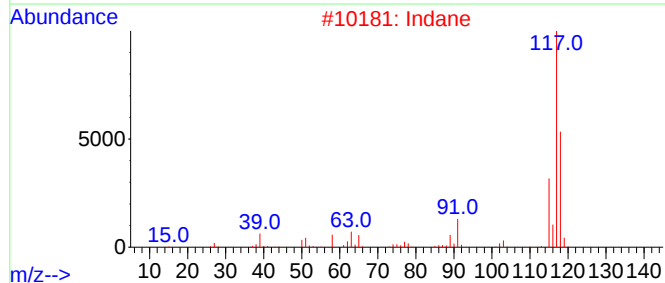
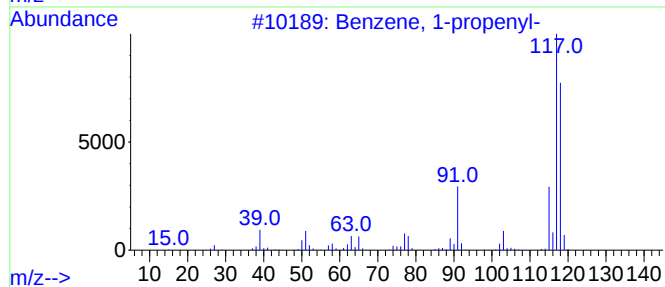
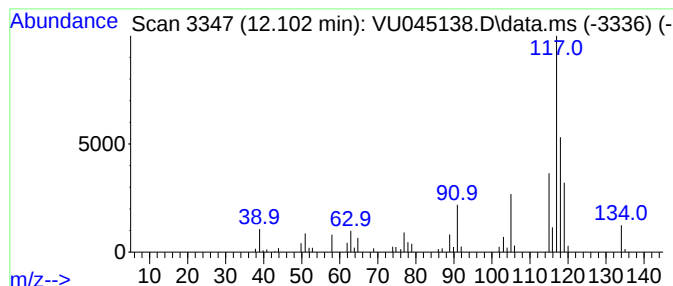
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Benzene, 1-propenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.102	3.47 ug/L	61628	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-propenyl-	118	C9H10	000637-50-3	93
2			Indane	118	C9H10	000496-11-7	91
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	86
4			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	70
5			Benzene, 1-propenyl-	118	C9H10	000637-50-3	70



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ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW8Z3ME

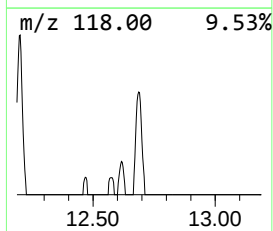
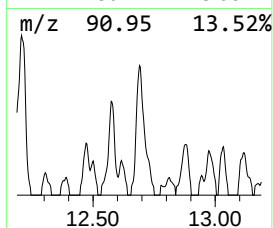
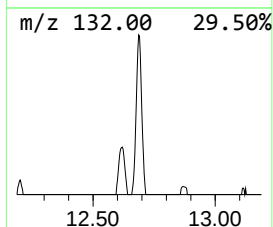
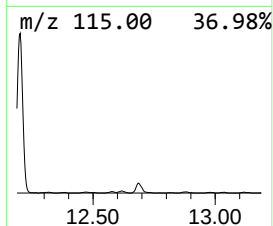
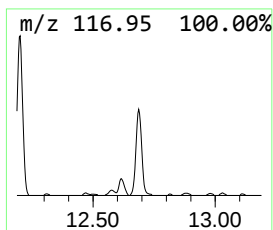
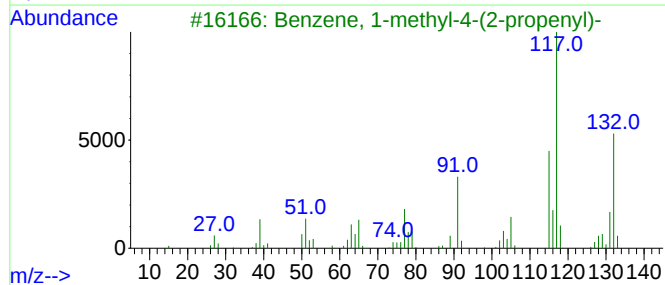
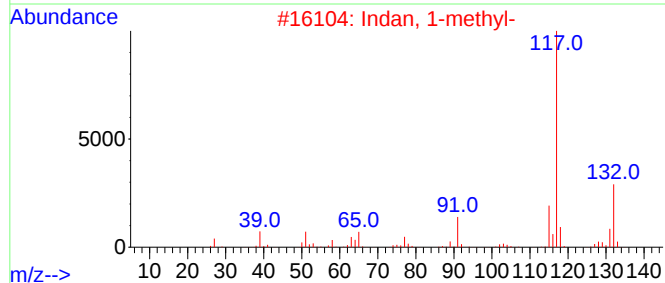
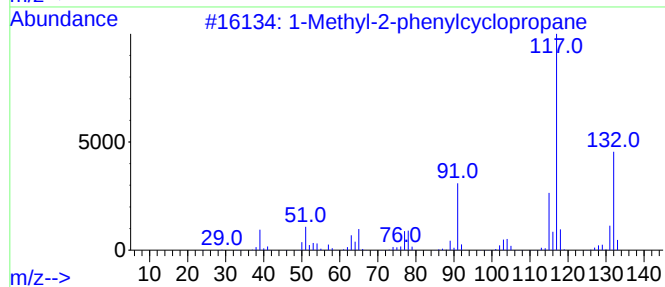
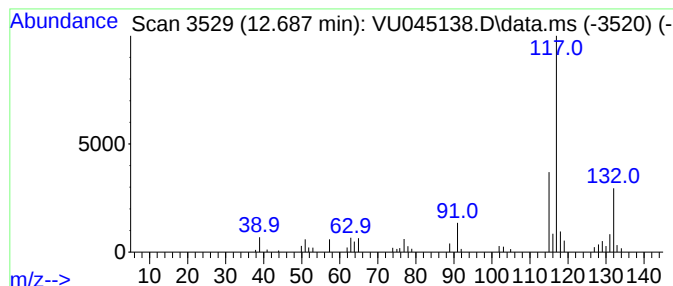
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Quant Title : VOC Analysis

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

Peak Number 4 1-Methyl-2-phenylcyclopropane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.687	3.73 ug/L	66306	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	87
2			Indan, 1-methyl-	132	C10H12	000767-58-8	87
3			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	83
4			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	83
5			Indan, 1-methyl-	132	C10H12	000767-58-8	81



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100521\
Data File : VU045138.D
Acq On : 05 Oct 2021 12:37
Operator : SY/MD
Sample : M3974-09ME
Misc : 5.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW8Z3ME

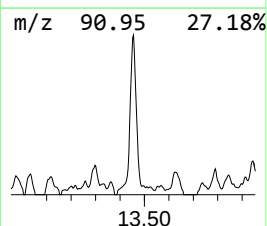
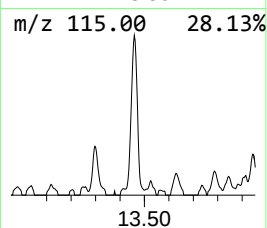
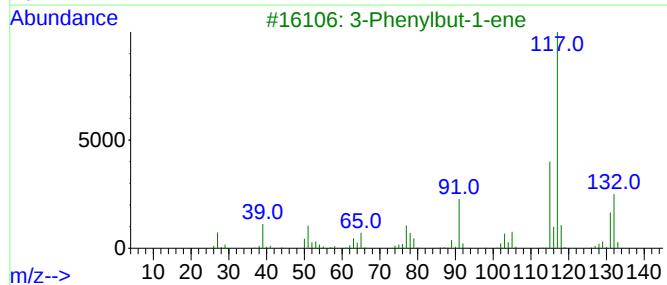
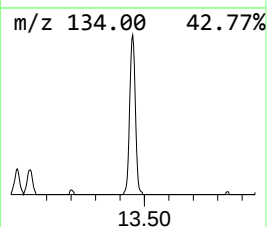
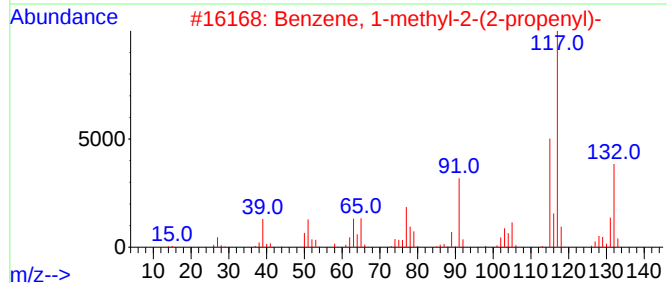
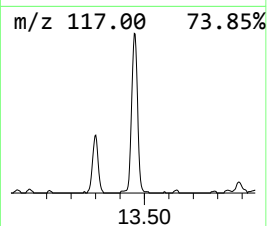
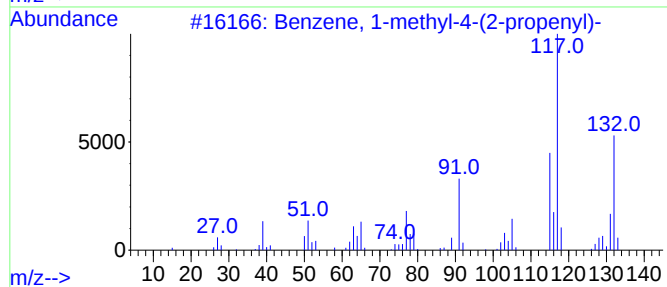
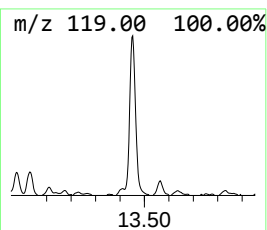
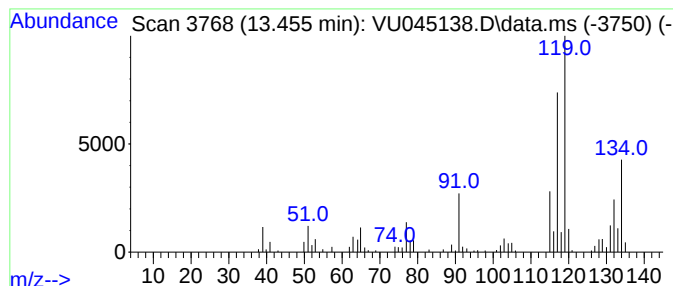
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Quant Title : VOC Analysis

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

Peak Number 5 Benzene, 1-methyl-4-(2-prop... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.455	8.49 ug/L	150692	1,4-Dichlorobenzene-d4	11.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	64
2			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	64
3			3-Phenylbut-1-ene	132	C10H12	000934-10-1	50
4			Benzene, 1-methyl-3-(1-methyleth...)	134	C10H14	000535-77-3	50
5			1-Phenyl-1-butene	132	C10H12	000824-90-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100521\
Data File : VU045138.D
Acq On : 05 Oct 2021 12:37
Operator : SY/MD
Sample : M3974-09ME
Misc : 5.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW8Z3ME

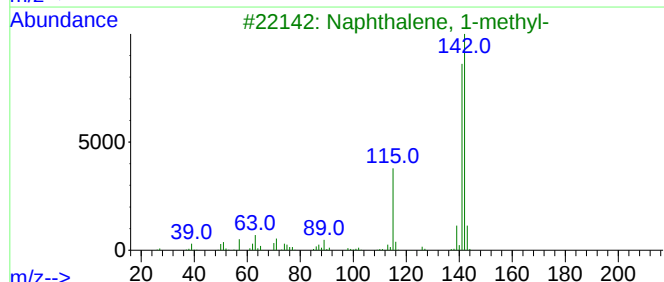
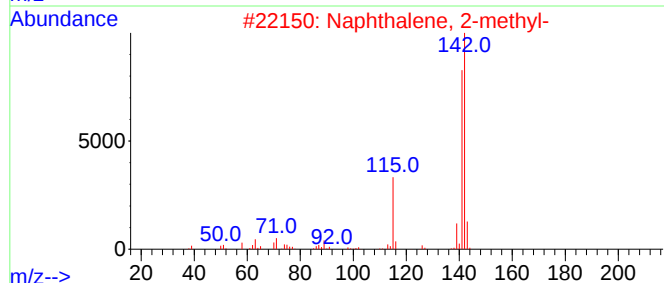
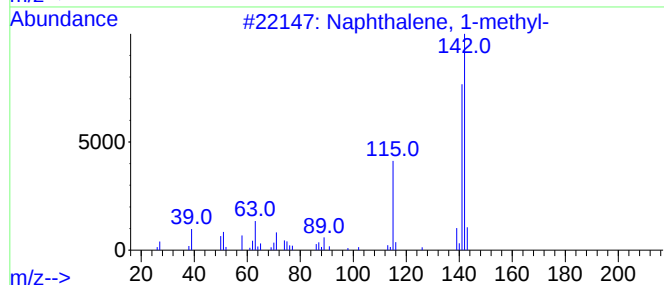
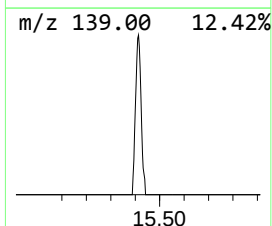
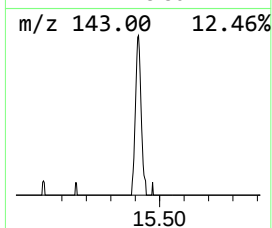
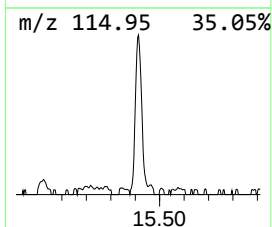
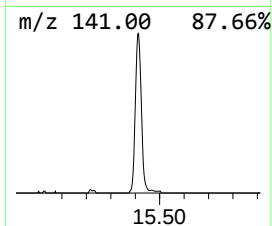
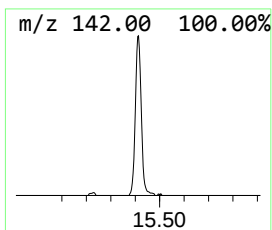
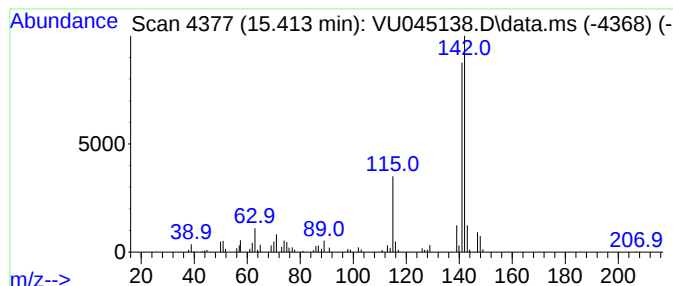
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Quant Title : VOC Analysis

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

Peak Number 6 Naphthalene, 1-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.413	4.65 ug/L	82627	1,4-Dichlorobenzene-d4	11.822

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, 1-methyl-	142	C11H10	000090-12-0	96
4			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
5			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100521\
Data File : VU045138.D
Acq On : 05 Oct 2021 12:37
Operator : SY/MD
Sample : M3974-09ME
Misc : 5.08g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 6 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW8Z3ME

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, 1-ethy...	11.298	3.0	ug/L	52985	3	11.822	887703	50.0
Benzene, 1-prop...	12.102	3.5	ug/L	61628	3	11.822	887703	50.0
1-Methyl-2-phen...	12.687	3.7	ug/L	66306	3	11.822	887703	50.0
Benzene, 1-meth...	13.455	8.5	ug/L	150692	3	11.822	887703	50.0
Naphthalene, 1-...	15.413	4.7	ug/L	82627	3	11.822	887703	50.0