

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062124\
 Data File : VU059409.D
 Acq On : 21 Jun 2024 13:33
 Operator : MD/SY
 Sample : P2962-06 100X
 Misc : 4.52g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0T78

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\SFAMULM052924WMA.M
 Title : VOC Analysis

Signal : TIC: VU059409.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.595	87	95	108	rBV	59628	71545	5.44%	0.825%
2	1.769	142	149	161	rVB3	11973	17047	1.30%	0.197%
3	1.904	184	191	211	rVB	52852	74883	5.69%	0.863%
4	2.264	297	303	305	rBV5	892	1018	0.08%	0.012%
5	2.560	383	395	413	rBV	101862	166418	12.65%	1.919%
6	2.775	458	462	466	rBV2	444	465	0.04%	0.005%
7	2.865	478	490	494	rBV2	585	1001	0.08%	0.012%
8	3.039	534	544	555	rVB5	3787	6987	0.53%	0.081%
9	3.328	629	634	641	rVB2	225	339	0.03%	0.004%
10	3.496	679	686	690	rBV2	250	320	0.02%	0.004%
11	3.914	808	816	819	rBV2	215	307	0.02%	0.004%
12	4.615	1021	1034	1059	rBV	73670	178978	13.61%	2.064%
13	5.055	1154	1171	1196	rBV	112619	251428	19.12%	2.899%
14	5.309	1245	1250	1254	rBV2	411	457	0.03%	0.005%
15	5.717	1351	1377	1407	rBV2	220318	607095	46.16%	7.001%
16	6.242	1524	1540	1567	rBV	299474	574215	43.66%	6.621%
17	6.528	1621	1629	1642	rVB6	4302	7835	0.60%	0.090%
18	6.685	1664	1678	1700	rBV2	141158	277742	21.12%	3.203%
19	6.762	1700	1702	1708	rVV3	593	595	0.05%	0.007%
20	7.193	1829	1836	1844	rBV2	1823	2937	0.22%	0.034%
21	7.563	1939	1951	1970	rBV2	69022	126282	9.60%	1.456%
22	7.711	1987	1997	2002	rBV3	1274	2179	0.17%	0.025%
23	7.750	2007	2009	2014	rVB2	581	384	0.03%	0.004%
24	7.894	2041	2054	2069	rBV	252373	440778	33.51%	5.083%
25	7.968	2072	2077	2088	rVB2	10730	16987	1.29%	0.196%
26	8.177	2129	2142	2161	rBV	47696	82307	6.26%	0.949%
27	8.264	2166	2169	2172	rVV2	526	385	0.03%	0.004%
28	8.553	2247	2259	2269	rBV5	3992	6555	0.50%	0.076%
29	8.627	2269	2282	2319	rBV	192072	370591	28.18%	4.273%
30	9.328	2496	2500	2504	rVB4	473	375	0.03%	0.004%
31	9.412	2513	2526	2564	rBV	433460	730750	55.56%	8.426%
32	9.566	2564	2574	2590	rVB	75143	123032	9.35%	1.419%
33	9.692	2603	2613	2627	rVV	56008	95639	7.27%	1.103%
34	10.016	2709	2714	2721	rVB3	730	751	0.06%	0.009%
35	10.097	2729	2739	2755	rBV	27891	47687	3.63%	0.550%
36	10.251	2778	2787	2796	rVV5	3174	4555	0.35%	0.053%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
 Title : VOC Analysis

37	10.315	2803	2807	2811	rVB2	420	401	0.03%	0.005%
38	10.347	2811	2817	2824	rBV6	1488	2287	0.17%	0.026%
39	10.386	2826	2829	2830	rBV	860	388	0.03%	0.004%
40	10.483	2850	2859	2872	rVB	6244	9995	0.76%	0.115%
41	10.560	2872	2883	2891	rBV7	1951	3663	0.28%	0.042%
42	10.614	2895	2900	2901	rBV3	1977	1340	0.10%	0.015%
43	10.749	2930	2942	2958	rBV	236643	382164	29.06%	4.407%
44	10.907	2981	2991	3001	rBV2	2778	4506	0.34%	0.052%
45	10.994	3008	3018	3024	rBV	49723	83728	6.37%	0.965%
46	11.084	3040	3046	3060	rVB2	13391	21496	1.63%	0.248%
47	11.235	3088	3093	3096	rBV2	530	432	0.03%	0.005%
48	11.290	3102	3110	3116	rBV4	3771	6267	0.48%	0.072%
49	11.373	3128	3136	3137	rBV3	970	1063	0.08%	0.012%
50	11.412	3141	3148	3154	rVV3	6220	8727	0.66%	0.101%
51	11.466	3155	3165	3178	rVB	41204	68129	5.18%	0.786%
52	11.537	3178	3187	3199	rBV	18657	30259	2.30%	0.349%
53	11.708	3232	3240	3244	rBV6	2018	3191	0.24%	0.037%
54	11.740	3245	3250	3258	rVB2	3490	5204	0.40%	0.060%
55	11.807	3258	3271	3287	rBV	449556	736808	56.02%	8.496%
56	11.891	3291	3297	3309	rVV	13945	23595	1.79%	0.272%
57	11.952	3309	3316	3325	rVV5	6460	9036	0.69%	0.104%
58	12.090	3349	3359	3373	rBV3	13672	23531	1.79%	0.271%
59	12.187	3377	3389	3407	rBV	290392	479089	36.42%	5.524%
60	12.309	3417	3427	3444	rVB	107662	175109	13.31%	2.019%
61	12.466	3468	3476	3477	rBV3	1112	1152	0.09%	0.013%
62	12.492	3482	3484	3492	rVB4	2177	1724	0.13%	0.020%
63	12.569	3499	3508	3517	rBV	10610	15347	1.17%	0.177%
64	12.630	3519	3527	3534	rVB5	2990	4148	0.32%	0.048%
65	12.749	3553	3564	3574	rBV3	12486	19883	1.51%	0.229%
66	12.810	3576	3583	3597	rVB6	3160	4726	0.36%	0.054%
67	12.871	3597	3602	3611	rBV3	716	1061	0.08%	0.012%
68	12.965	3626	3631	3640	rVV3	1926	2615	0.20%	0.030%
69	13.026	3642	3650	3659	rBV3	4594	6994	0.53%	0.081%
70	13.097	3664	3672	3678	rBV6	1218	1358	0.10%	0.016%
71	13.164	3685	3693	3700	rBV6	2095	3423	0.26%	0.039%
72	13.199	3702	3704	3709	rVB3	986	813	0.06%	0.009%
73	13.228	3709	3713	3718	rBV3	516	497	0.04%	0.006%
74	13.293	3726	3733	3740	rVB5	2153	3145	0.24%	0.036%
75	13.447	3766	3781	3793	rBV6	5325	10688	0.81%	0.123%
76	13.518	3793	3803	3814	rBV4	25773	40290	3.06%	0.465%

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77	13.624	3825	3836	3852	rVB	27402	47411	3.60%	0.547%
78	13.691	3852	3857	3858	rBV3	1144	887	0.07%	0.010%
79	13.727	3861	3868	3876	rVB3	3629	5496	0.42%	0.063%
80	13.833	3899	3901	3905	rVV3	610	504	0.04%	0.006%
81	14.080	3964	3978	4005	rBV	817626	1315288	100.00%	15.167%
82	14.206	4008	4017	4028	rVB	9831	17116	1.30%	0.197%
83	14.415	4079	4082	4085	rBV	459	338	0.03%	0.004%
84	14.444	4087	4091	4099	rVB4	1496	1877	0.14%	0.022%
85	14.511	4108	4112	4123	rVB6	864	1564	0.12%	0.018%
86	14.675	4154	4163	4170	rBV7	3189	5175	0.39%	0.060%
87	14.772	4188	4193	4194	rBV	520	473	0.04%	0.005%
88	14.926	4236	4241	4250	rVB5	1639	2608	0.20%	0.030%
89	15.071	4280	4286	4294	rVB6	1811	2612	0.20%	0.030%
90	15.167	4309	4316	4320	rBV3	2316	3213	0.24%	0.037%
91	15.219	4321	4332	4360	rVB	237672	381013	28.97%	4.394%
92	15.334	4360	4368	4378	rBV4	2547	4029	0.31%	0.046%
93	15.405	4378	4390	4404	rBV	131809	218122	16.58%	2.515%
94	15.550	4432	4435	4437	rVB2	704	444	0.03%	0.005%
95	15.952	4551	4560	4573	rBV2	18055	28850	2.19%	0.333%
96	16.145	4612	4620	4627	rBV2	14696	21669	1.65%	0.250%
97	16.260	4647	4656	4679	rVB3	22214	40129	3.05%	0.463%
98	16.405	4692	4701	4708	rBV2	28579	43937	3.34%	0.507%
99	16.547	4739	4745	4756	rVB8	5221	9093	0.69%	0.105%
100	16.884	4842	4850	4862	rVB3	19188	31183	2.37%	0.360%

Sum of corrected areas: 8672152

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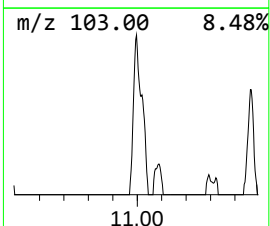
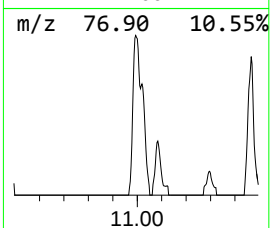
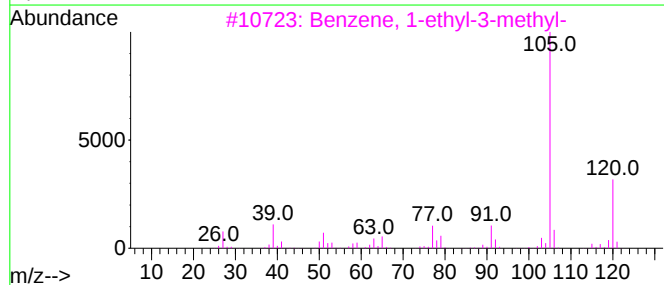
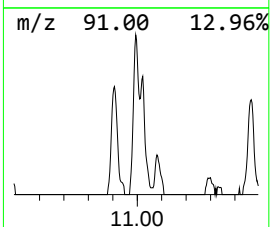
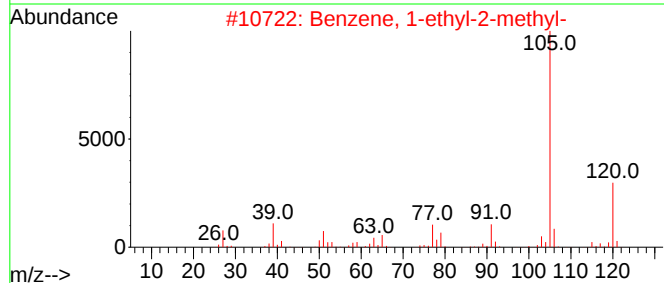
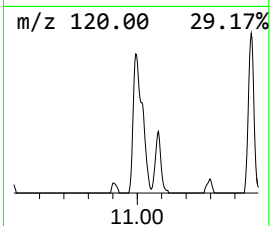
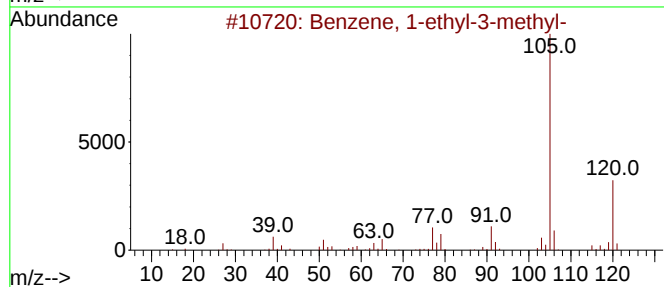
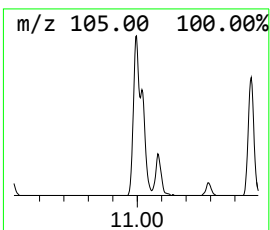
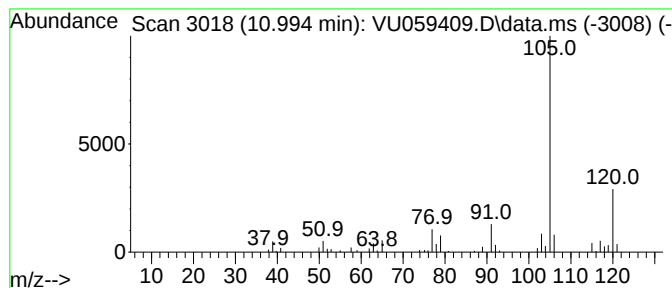
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Benzene, 1-ethyl-3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.994	5.68 ug/L	83728	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	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-4-methyl-	120	C9H12	000622-96-8	94
5			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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Instrument :
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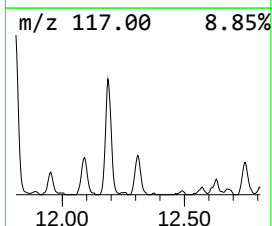
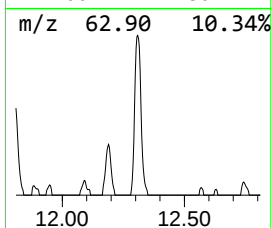
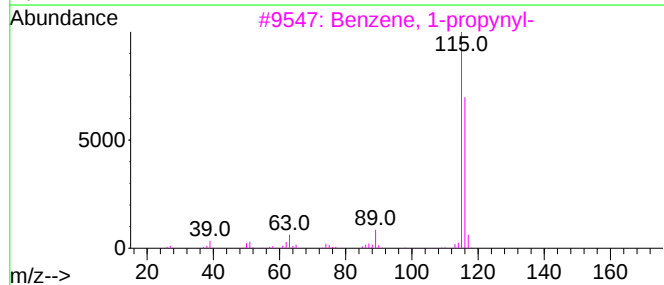
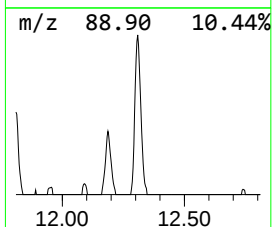
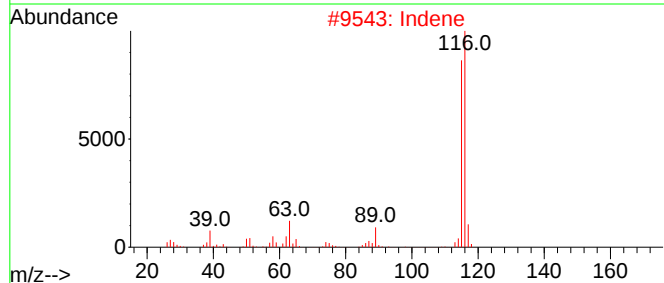
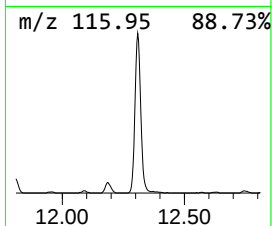
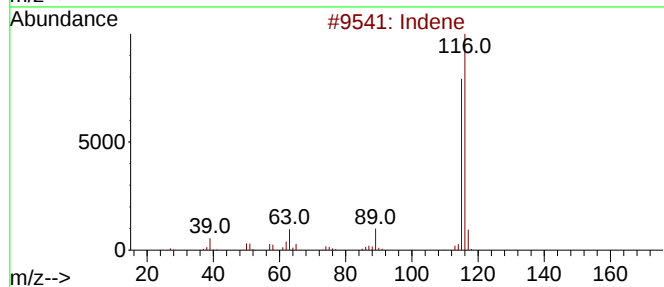
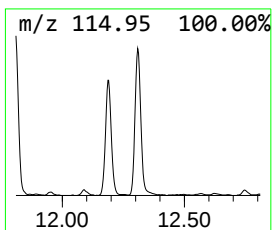
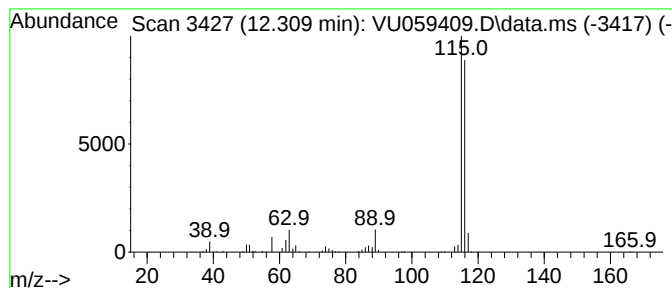
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Indene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.309	11.88 ug/L	175109	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene			116	C9H8	000095-13-6	97
2	Indene			116	C9H8	000095-13-6	95
3	Benzene, 1-propynyl-			116	C9H8	000673-32-5	94
4	Indene			116	C9H8	000095-13-6	94
5	Benzene, 1-propynyl-			116	C9H8	000673-32-5	91



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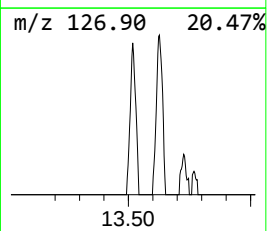
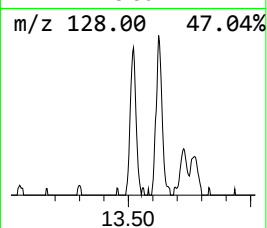
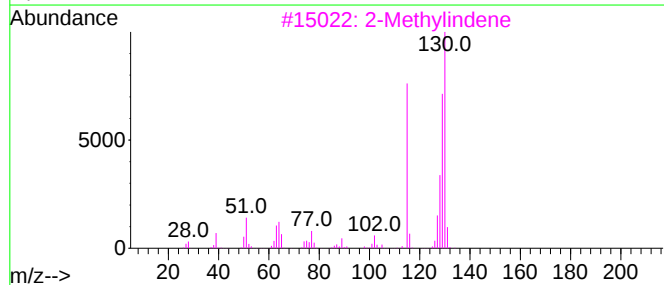
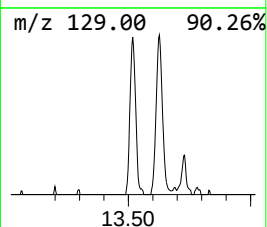
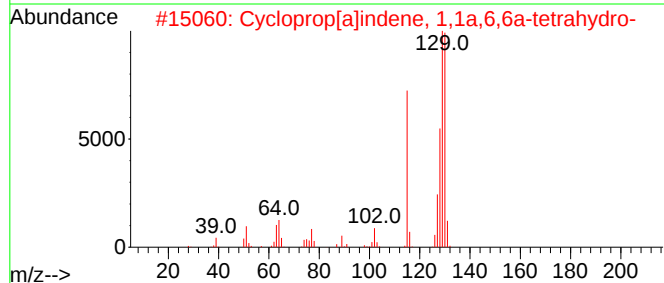
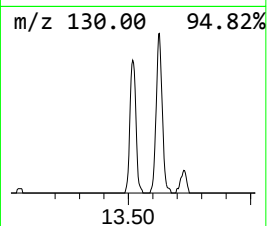
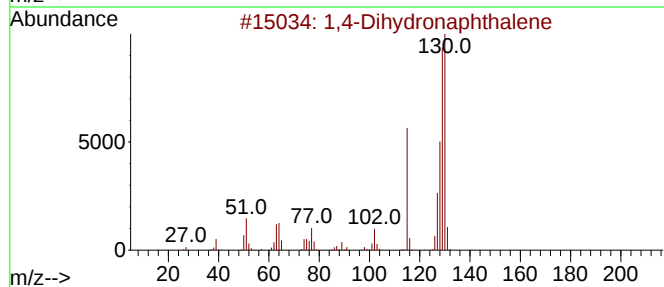
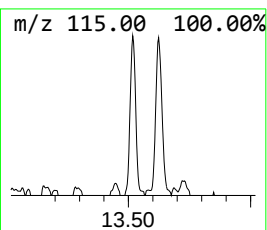
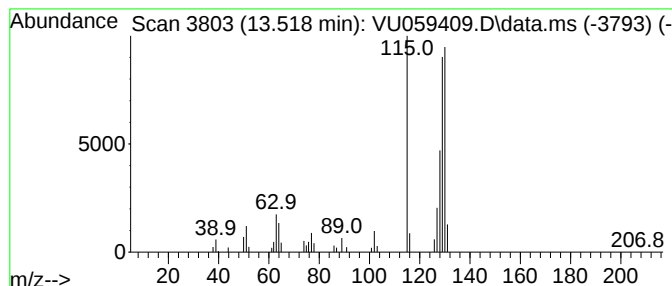
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 1,4-Dihydronaphthalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.518	2.73 ug/L	40290	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Dihydronaphthalene	130	C10H10	000612-17-9	95
2			Cycloprop[a]indene, 1,1a,6,6a-te...	130	C10H10	015677-15-3	95
3			2-Methylindene	130	C10H10	002177-47-1	93
4			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	93
5			Benzene, 1-butynyl-	130	C10H10	000622-76-4	91



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Operator : MD/SY
Sample : P2962-06 100X
Misc : 4.52g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0T78

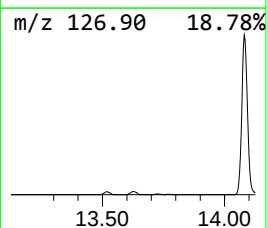
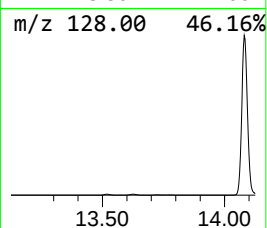
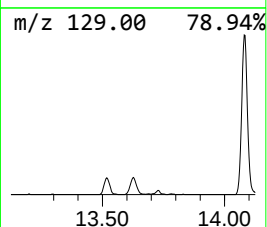
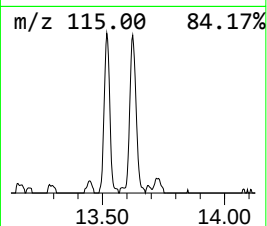
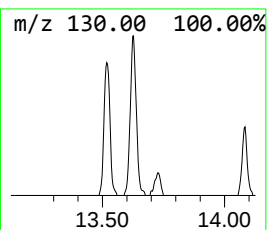
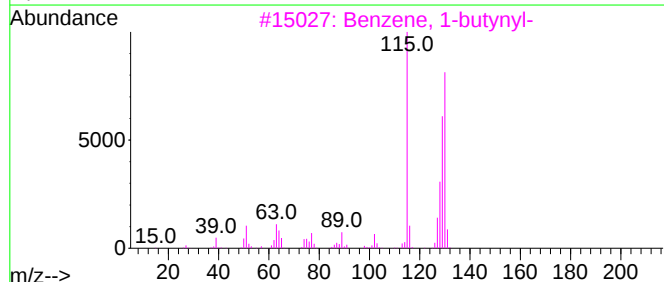
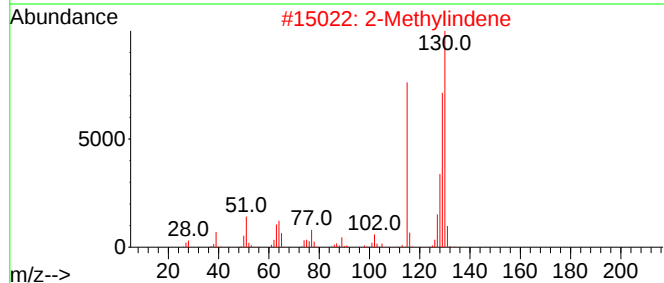
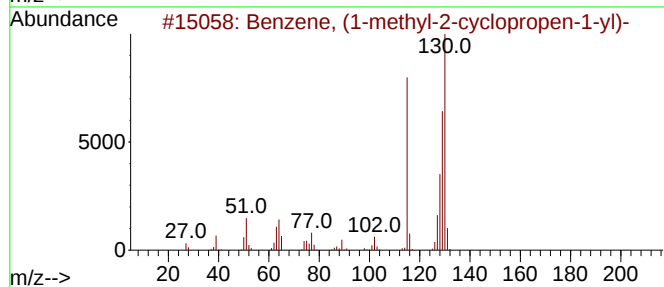
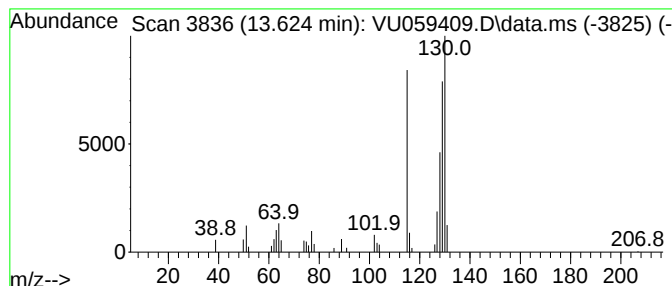
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Quant Title : VOC Analysis

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

Peak Number 5 Benzene, (1-methyl-2-cyclop... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.624	3.22 ug/L	47411	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methyl-2-cyclopropen...	130	C10H10	065051-83-4	95
2			2-Methylindene	130	C10H10	002177-47-1	95
3			Benzene, 1-butyryl-	130	C10H10	000622-76-4	95
4			Naphthalene, 1,2-dihydro-	130	C10H10	000447-53-0	93
5			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062124\
Data File : VU059409.D
Acq On : 21 Jun 2024 13:33
Operator : MD/SY
Sample : P2962-06 100X
Misc : 4.52g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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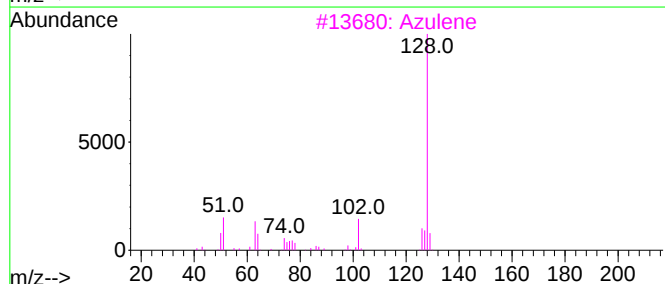
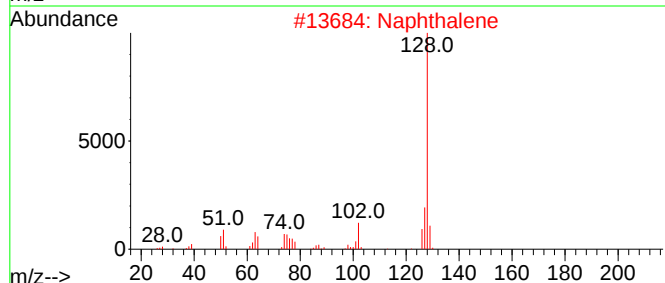
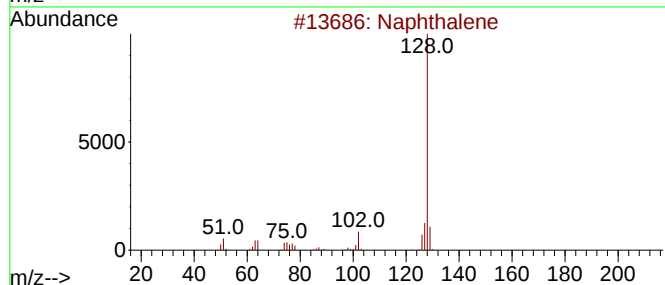
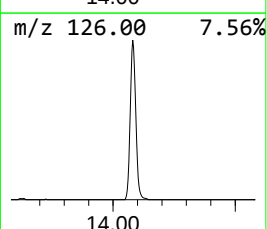
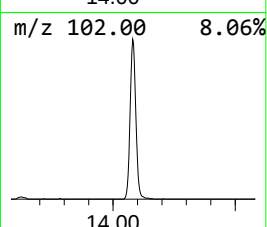
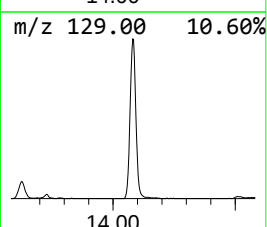
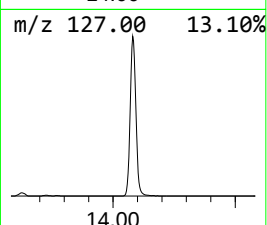
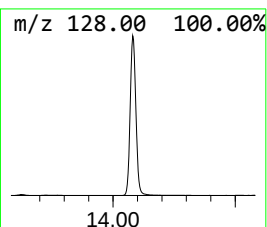
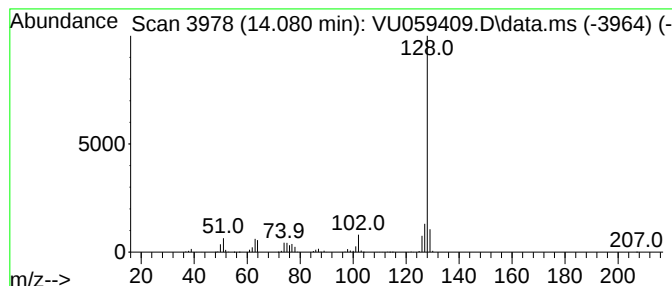
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Quant Title : VOC Analysis

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

Peak Number 6 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.081	89.26 ug/L	1315290	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Naphthalene	128	C10H8	000091-20-3	94
3			Azulene	128	C10H8	000275-51-4	91
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	90



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062124\
Data File : VU059409.D
Acq On : 21 Jun 2024 13:33
Operator : MD/SY
Sample : P2962-06 100X
Misc : 4.52g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0T78

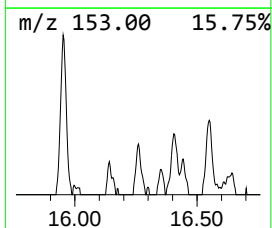
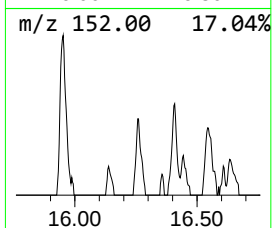
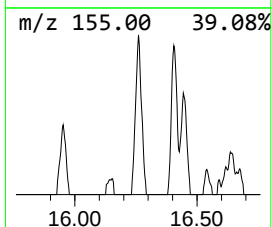
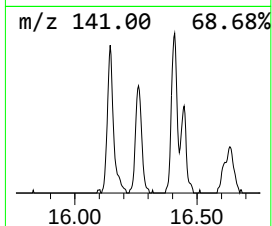
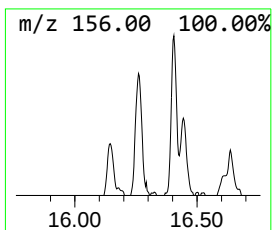
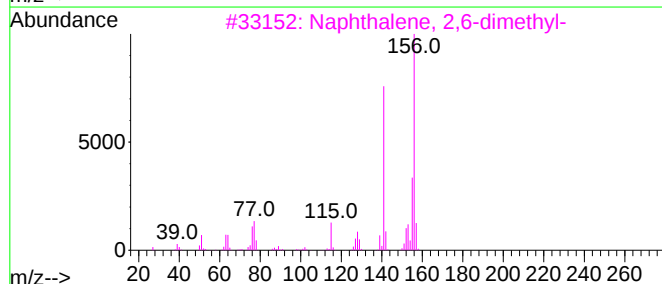
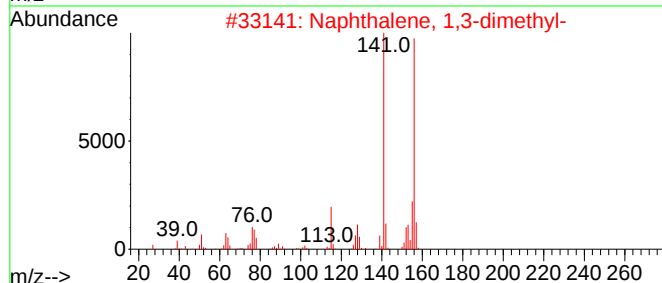
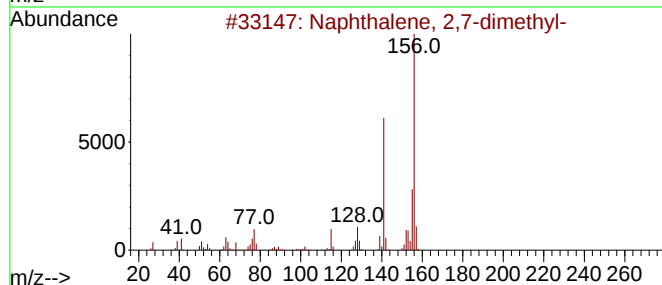
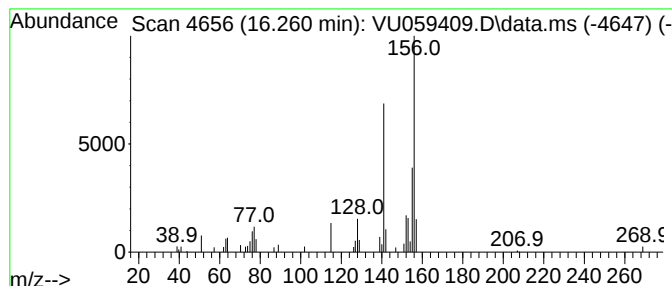
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Quant Title : VOC Analysis

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

Peak Number 9 Naphthalene, 2,7-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.260	2.72 ug/L	40129	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96
2			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
3			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	96
4			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96
5			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062124\
Data File : VU059409.D
Acq On : 21 Jun 2024 13:33
Operator : MD/SY
Sample : P2962-06 100X
Misc : 4.52g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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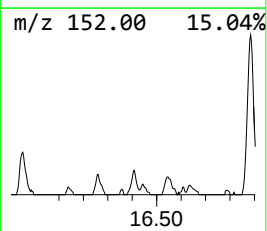
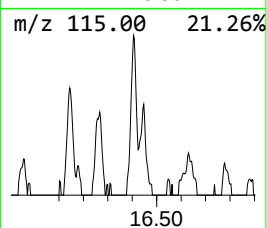
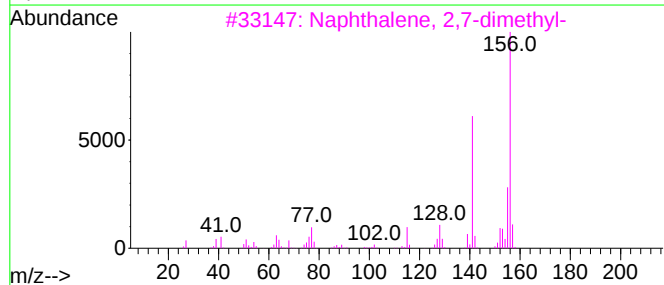
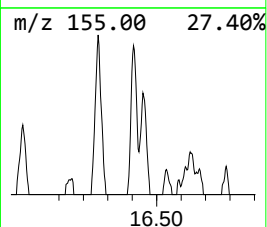
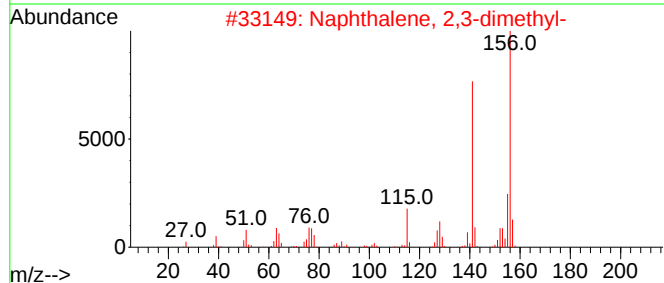
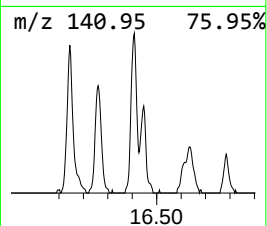
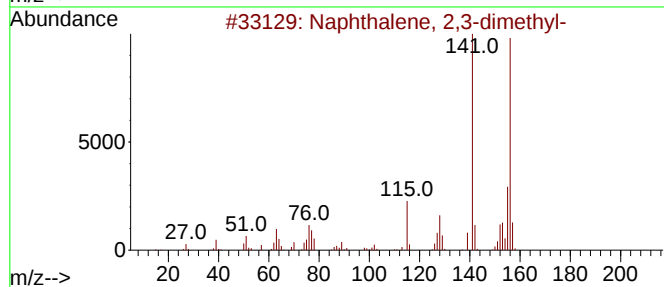
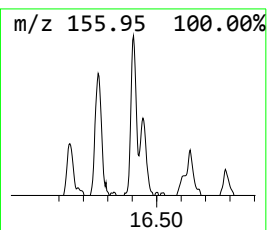
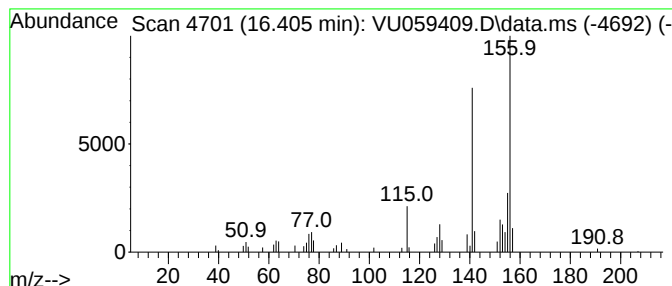
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Quant Title : VOC Analysis

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

Peak Number 10 Naphthalene, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.405	2.98 ug/L	43937	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
2			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	96
3			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	96
4			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
5			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062124\
Data File : VU059409.D
Acq On : 21 Jun 2024 13:33
Operator : MD/SY
Sample : P2962-06 100X
Misc : 4.52g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0T78

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.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...	10.994	5.7	ug/L	83728	3	11.807	736808	50.0
Indene	12.309	11.9	ug/L	175109	3	11.807	736808	50.0
1,4-Dihydronaph...	13.518	2.7	ug/L	40290	3	11.807	736808	50.0
Benzene, (1-met...	13.624	3.2	ug/L	47411	3	11.807	736808	50.0
Azulene	14.081	89.3	ug/L	1315290	3	11.807	736808	50.0
Naphthalene, 2,...	16.260	2.7	ug/L	40129	3	11.807	736808	50.0
Naphthalene, 2,...	16.405	3.0	ug/L	43937	3	11.807	736808	50.0