

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
 Data File : VU059333.D
 Acq On : 18 Jun 2024 23:48
 Operator : MD/SY
 Sample : P2873-09 200X
 Misc : 3.28g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0SJ9

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: VU059333.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.596	88	95	109	rBV	51898	61289	5.98%	0.923%
2	1.763	139	147	160	rBV	6672	10726	1.05%	0.162%
3	1.908	184	192	207	rBV	47171	65120	6.35%	0.981%
4	2.560	383	395	409	rVV	80838	133213	13.00%	2.007%
5	2.618	411	413	427	rVB3	966	1443	0.14%	0.022%
6	2.785	461	465	471	rVB2	329	380	0.04%	0.006%
7	2.946	508	515	517	rBV	238	330	0.03%	0.005%
8	3.036	531	543	558	rBV2	14543	27588	2.69%	0.416%
9	3.158	576	581	583	rBV	413	363	0.04%	0.005%
10	3.435	663	667	672	rBV2	296	376	0.04%	0.006%
11	3.486	680	683	690	rVB	371	390	0.04%	0.006%
12	3.936	818	823	825	rBV	296	283	0.03%	0.004%
13	4.042	849	856	857	rBV2	317	322	0.03%	0.005%
14	4.563	1015	1018	1023	rVB2	364	317	0.03%	0.005%
15	4.615	1023	1034	1064	rBV	51382	130575	12.74%	1.967%
16	5.055	1156	1171	1190	rVV	87414	193425	18.87%	2.914%
17	5.351	1260	1263	1269	rVB2	305	338	0.03%	0.005%
18	5.509	1306	1312	1315	rBV2	231	265	0.03%	0.004%
19	5.718	1357	1377	1400	rBV3	171192	474010	46.24%	7.141%
20	6.007	1456	1467	1468	rBV	196	347	0.03%	0.005%
21	6.094	1486	1494	1500	rBV2	254	384	0.04%	0.006%
22	6.245	1526	1541	1561	rBV	177321	347053	33.86%	5.229%
23	6.531	1621	1630	1639	rVB8	3922	6866	0.67%	0.103%
24	6.685	1664	1678	1698	rBV	111345	217344	21.20%	3.274%
25	7.197	1831	1837	1849	rBV5	1379	2385	0.23%	0.036%
26	7.303	1862	1870	1873	rBV2	280	469	0.05%	0.007%
27	7.563	1940	1951	1966	rBV2	47994	86491	8.44%	1.303%
28	7.689	1987	1990	1992	rBV2	409	295	0.03%	0.004%
29	7.714	1996	1998	2008	rVB4	657	747	0.07%	0.011%
30	7.894	2041	2054	2072	rBV	185752	322252	31.44%	4.855%
31	8.177	2132	2142	2159	rBV2	32959	57070	5.57%	0.860%
32	8.283	2171	2175	2181	rVB3	399	454	0.04%	0.007%
33	8.316	2181	2185	2190	rBV2	344	415	0.04%	0.006%
34	8.547	2243	2257	2273	rBV	479933	815682	79.57%	12.289%
35	8.627	2273	2282	2318	rVB	127968	256187	24.99%	3.860%
36	9.197	2456	2459	2468	rVB2	248	330	0.03%	0.005%

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Integrator: RTE

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

37	9.254	2468	2477	2481	rBV	250	427	0.04%	0.006%
38	9.412	2514	2526	2552	rBV	255653	440073	42.93%	6.630%
39	9.570	2566	2575	2588	rVB	15028	23708	2.31%	0.357%
40	9.692	2601	2613	2625	rBV	22831	39578	3.86%	0.596%
41	10.100	2730	2740	2758	rVB4	8971	18799	1.83%	0.283%
42	10.197	2767	2770	2775	rBV3	342	334	0.03%	0.005%
43	10.438	2843	2845	2849	rVB2	347	277	0.03%	0.004%
44	10.486	2854	2860	2861	rBV3	598	597	0.06%	0.009%
45	10.624	2901	2903	2909	rVB2	539	434	0.04%	0.007%
46	10.750	2927	2942	2964	rVV	168449	277071	27.03%	4.174%
47	10.907	2986	2991	3002	rVB2	1198	1896	0.18%	0.029%
48	11.000	3010	3020	3025	rBV3	6436	10700	1.04%	0.161%
49	11.087	3038	3047	3060	rVB	7591	12151	1.19%	0.183%
50	11.242	3090	3095	3100	rVV	276	324	0.03%	0.005%
51	11.287	3103	3109	3111	rVV2	1182	1153	0.11%	0.017%
52	11.319	3111	3119	3127	rVB6	3317	5642	0.55%	0.085%
53	11.467	3152	3165	3177	rVV	24414	37296	3.64%	0.562%
54	11.537	3177	3187	3196	rVV2	27156	42240	4.12%	0.636%
55	11.586	3197	3202	3216	rVV2	7860	12073	1.18%	0.182%
56	11.807	3259	3271	3291	rBV	255392	420903	41.06%	6.341%
57	11.891	3292	3297	3308	rVV2	7437	11301	1.10%	0.170%
58	11.952	3308	3316	3326	rVV5	3035	4984	0.49%	0.075%
59	12.094	3351	3360	3366	rBV4	3931	5982	0.58%	0.090%
60	12.190	3378	3390	3410	rBV	192987	316462	30.87%	4.768%
61	12.309	3416	3427	3446	rBV	30430	52190	5.09%	0.786%
62	12.492	3482	3484	3486	rBV3	474	298	0.03%	0.004%
63	12.547	3495	3501	3502	rBV2	1109	907	0.09%	0.014%
64	12.634	3520	3528	3537	rVB4	1243	2208	0.22%	0.033%
65	12.682	3540	3543	3550	rVB3	537	536	0.05%	0.008%
66	12.750	3555	3564	3576	rVV3	6763	10946	1.07%	0.165%
67	12.811	3577	3583	3592	rVB6	1395	2008	0.20%	0.030%
68	12.975	3626	3634	3642	rVB3	1030	1372	0.13%	0.021%
69	13.026	3643	3650	3656	rBV2	2366	3541	0.35%	0.053%
70	13.155	3682	3690	3703	rBV5	3540	5830	0.57%	0.088%
71	13.290	3729	3732	3739	rVB3	908	1088	0.11%	0.016%
72	13.447	3771	3781	3793	rVB10	3256	6064	0.59%	0.091%
73	13.518	3794	3803	3814	rBV4	12208	18034	1.76%	0.272%
74	13.627	3824	3837	3849	rBV4	12949	22431	2.19%	0.338%
75	13.695	3851	3858	3861	rBV2	517	643	0.06%	0.010%
76	13.724	3861	3867	3875	rVB4	1923	2345	0.23%	0.035%

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 Title : VOC Analysis

77	13.766	3877	3880	3883	rBV	411	319	0.03%	0.005%
78	13.839	3900	3903	3913	rVB4	695	835	0.08%	0.013%
79	13.952	3933	3938	3945	rBV	508	504	0.05%	0.008%
80	14.081	3965	3978	4006	rBV	635212	1025088	100.00%	15.444%
81	14.209	4008	4018	4029	rVB2	6271	11141	1.09%	0.168%
82	14.444	4086	4091	4097	rVV4	1173	1485	0.14%	0.022%
83	14.518	4109	4114	4119	rBV3	729	1101	0.11%	0.017%
84	14.679	4159	4164	4171	rVB5	1448	1680	0.16%	0.025%
85	14.807	4197	4204	4213	rBV8	1923	3355	0.33%	0.051%
86	14.929	4237	4242	4249	rVB4	1003	1394	0.14%	0.021%
87	15.016	4265	4269	4270	rBV3	462	346	0.03%	0.005%
88	15.071	4279	4286	4292	rBV4	1639	2318	0.23%	0.035%
89	15.171	4311	4317	4320	rBV	1446	1574	0.15%	0.024%
90	15.219	4321	4332	4354	rVB	172927	286023	27.90%	4.309%
91	15.405	4379	4390	4407	rBV	111633	185645	18.11%	2.797%
92	15.569	4433	4441	4445	rBV6	658	987	0.10%	0.015%
93	15.955	4552	4561	4569	rBV3	9974	16086	1.57%	0.242%
94	16.061	4591	4594	4597	rBV3	712	612	0.06%	0.009%
95	16.093	4602	4604	4606	rBV2	570	314	0.03%	0.005%
96	16.145	4615	4620	4627	rBV6	2391	2761	0.27%	0.042%
97	16.261	4646	4656	4664	rBV2	12787	21792	2.13%	0.328%
98	16.409	4693	4702	4709	rBV3	18103	27793	2.71%	0.419%
99	16.781	4815	4818	4825	rVB6	2709	2769	0.27%	0.042%
100	16.891	4845	4852	4863	rVB3	6898	11214	1.09%	0.169%

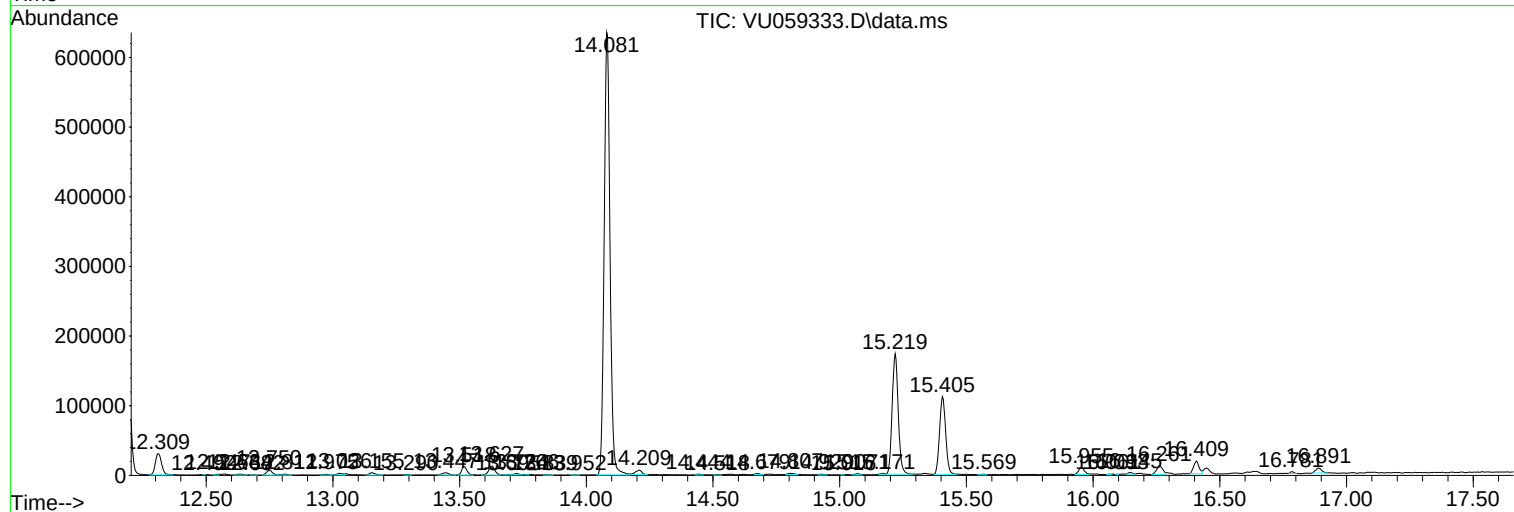
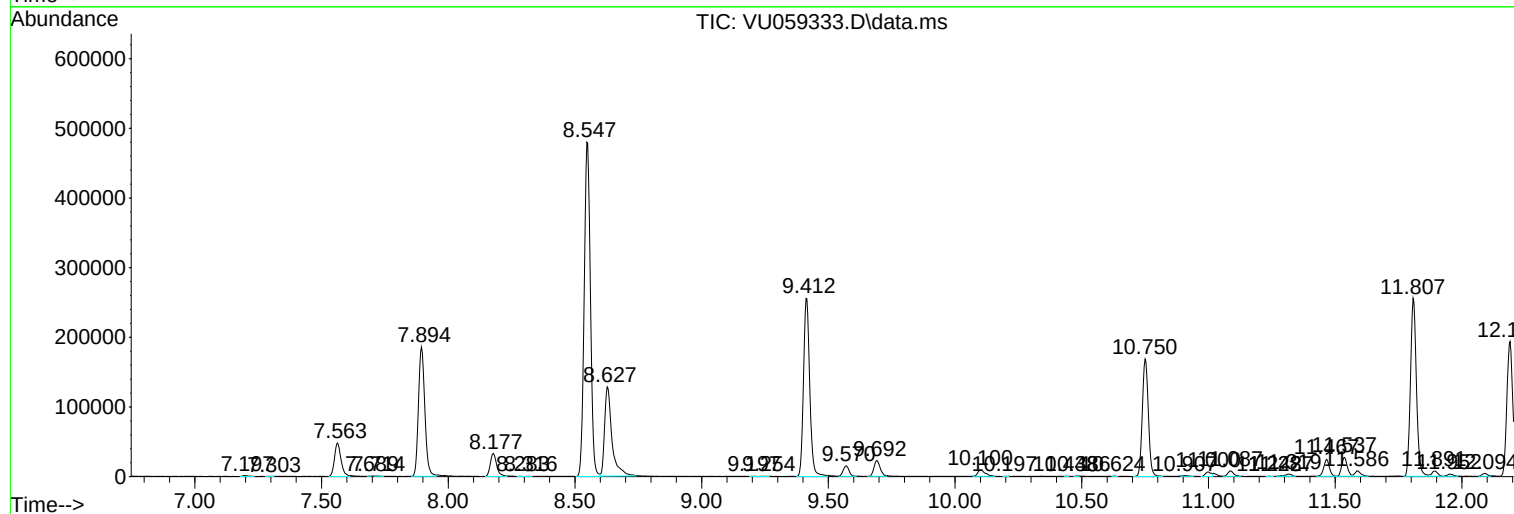
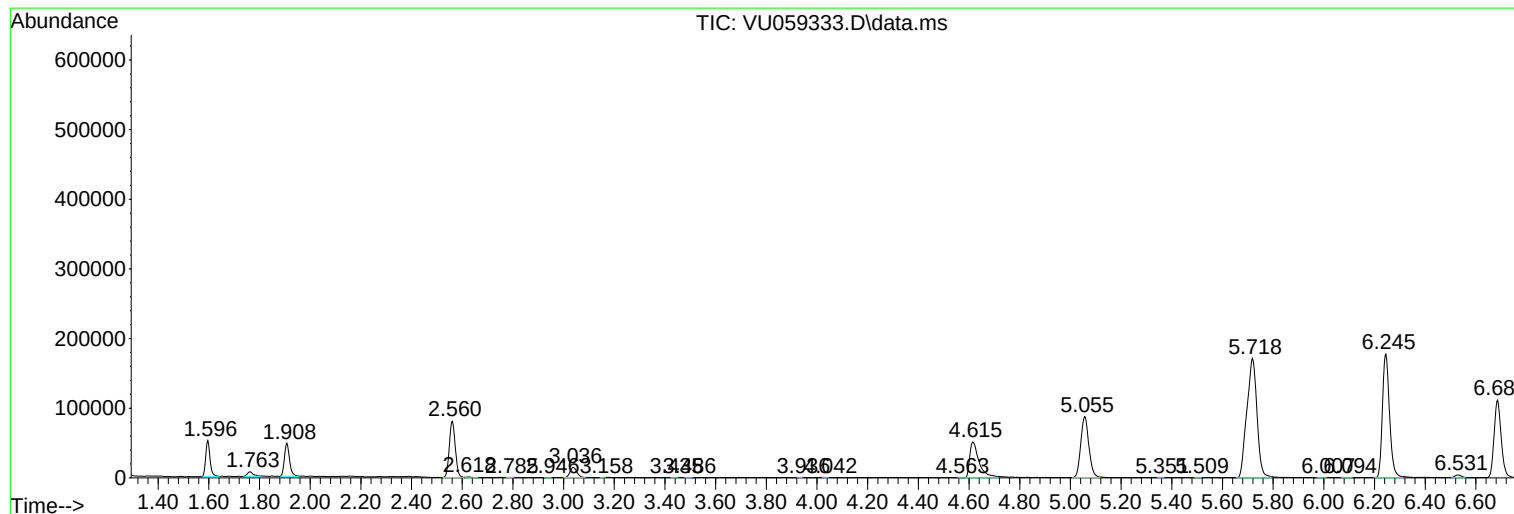
Sum of corrected areas: 6637506

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Instrument :
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ClientSampleId :
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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



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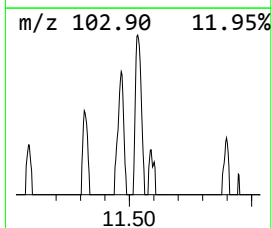
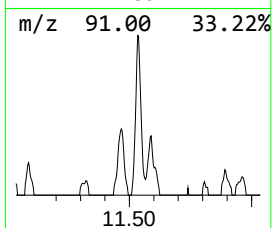
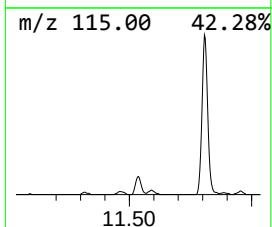
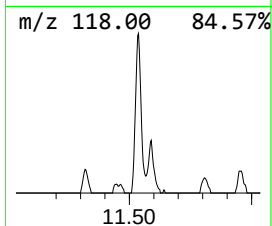
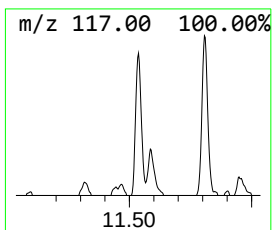
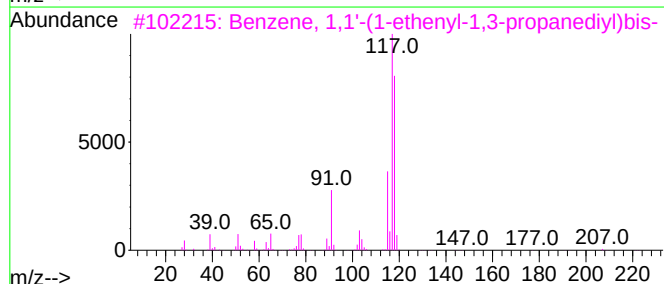
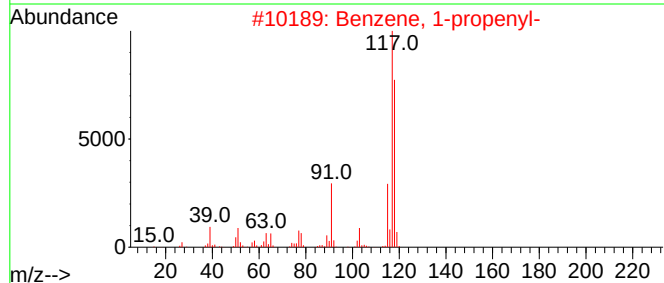
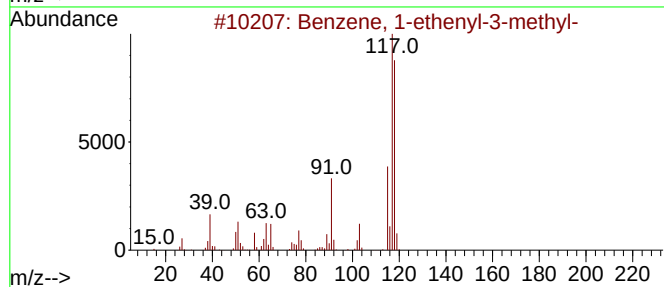
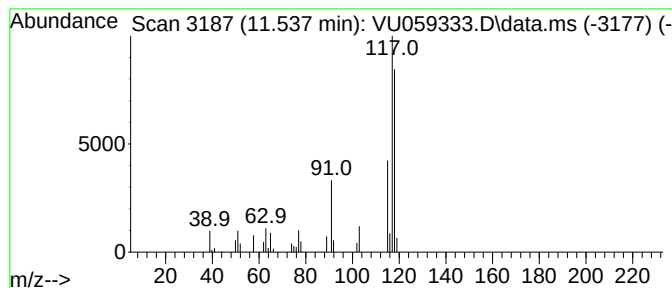
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.537	5.02 ug/L	42240	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	96
2			Benzene, 1-propenyl-	118	C9H10	000637-50-3	93
3			Benzene, 1,1'-(1-ethenyl-1,3-pro...	222	C17H18	061141-97-7	90
4			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	81
5			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81



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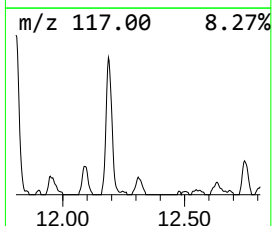
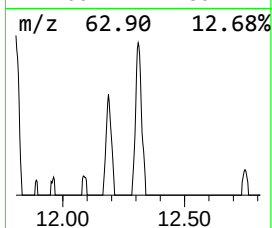
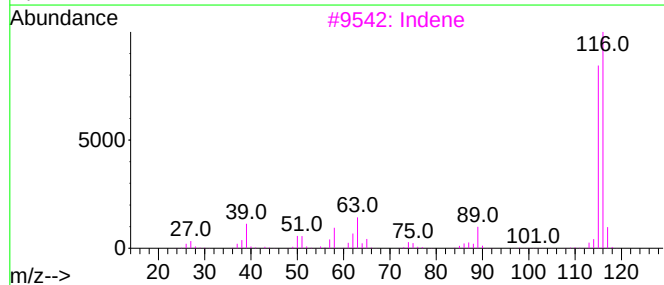
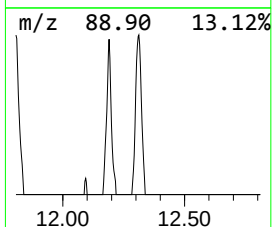
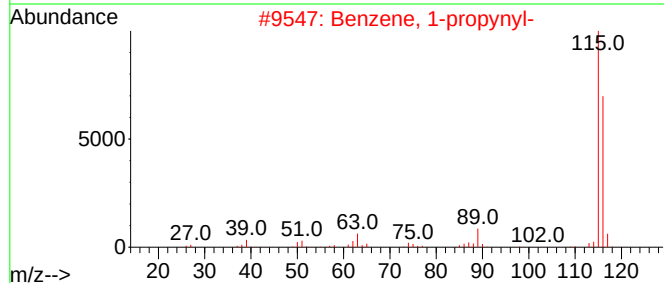
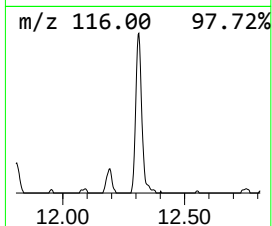
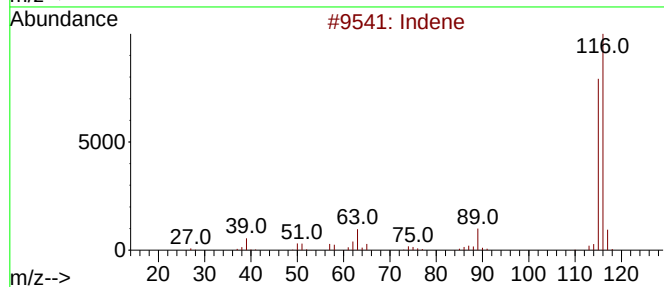
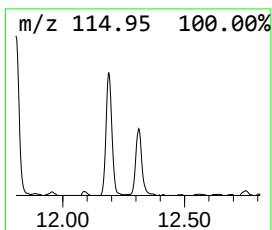
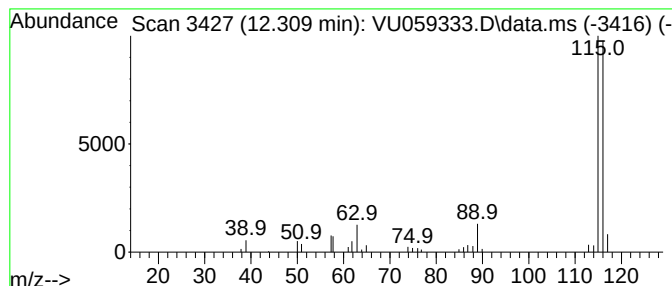
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Indene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.309	6.20 ug/L	52190	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indene	116	C9H8	000095-13-6	97
2			Benzene, 1-propynyl-	116	C9H8	000673-32-5	95
3			Indene	116	C9H8	000095-13-6	94
4			3-Methylphenylacetylene	116	C9H8	000766-82-5	91
5			Benzene, 1-propynyl-	116	C9H8	000673-32-5	91



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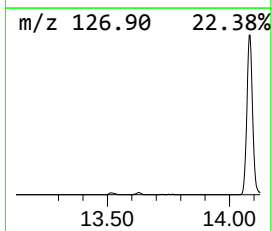
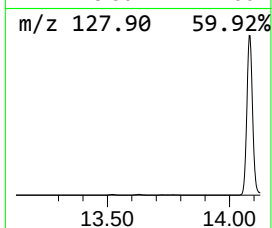
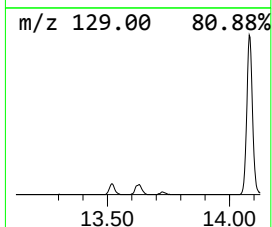
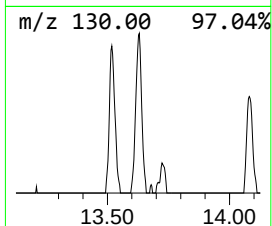
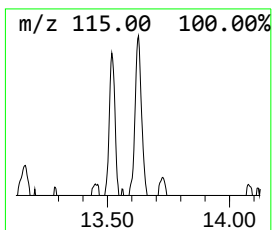
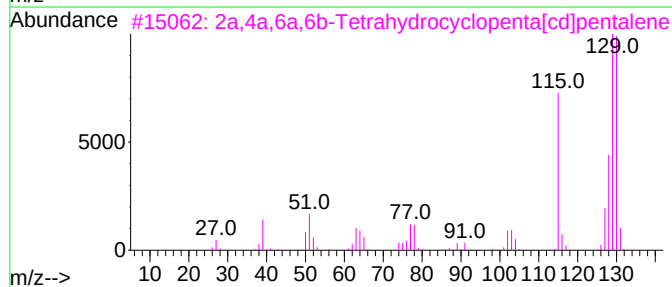
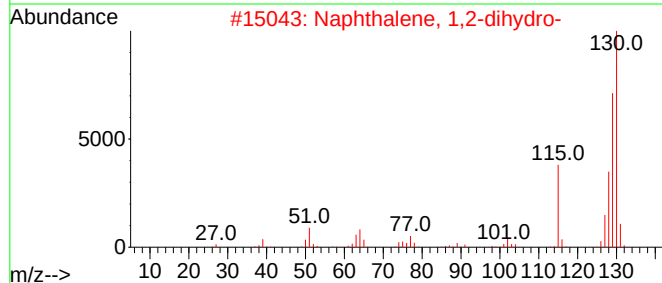
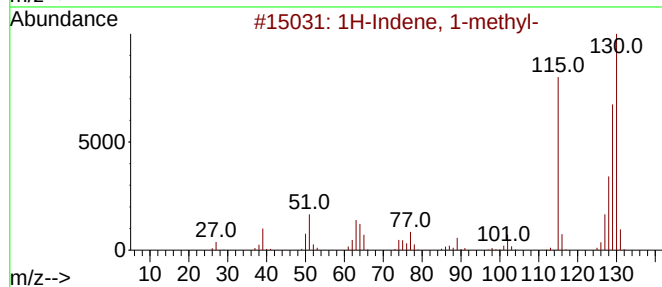
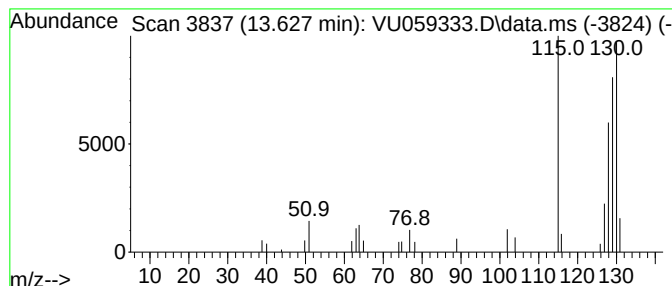
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Quant Title : VOC Analysis

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

Peak Number 4 1H-Indene, 1-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.627	2.66 ug/L	22431	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indene, 1-methyl-	130	C10H10	000767-59-9	91
2			Naphthalene, 1,2-dihydro-	130	C10H10	000447-53-0	91
3			2a,4a,6a,6b-Tetrahydrocyclopenta...	130	C10H10	006053-74-3	89
4			2-Methylindene	130	C10H10	002177-47-1	87
5			1H-Indene, 3-methyl-	130	C10H10	000767-60-2	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
Data File : VU059333.D
Acq On : 18 Jun 2024 23:48
Operator : MD/SY
Sample : P2873-09 200X
Misc : 3.28g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SJ9

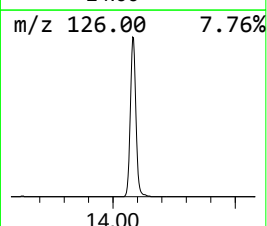
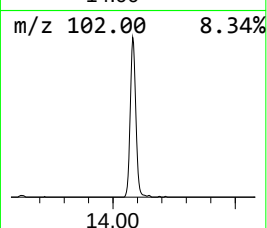
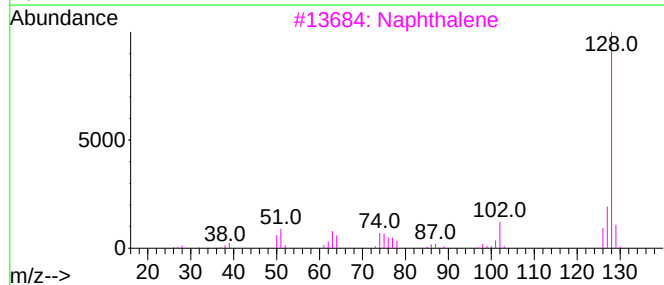
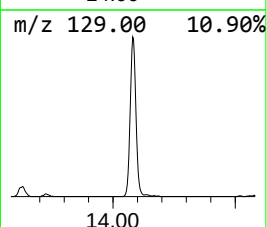
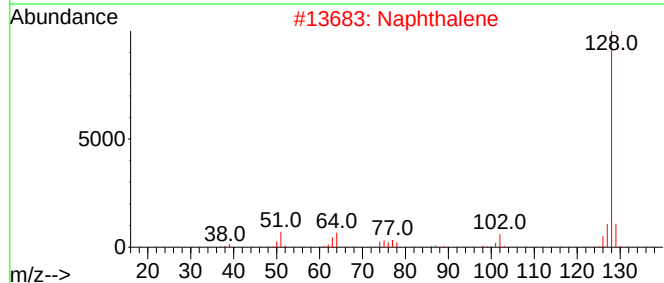
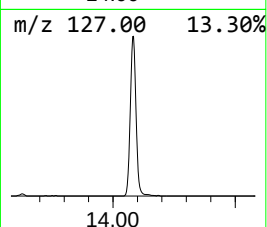
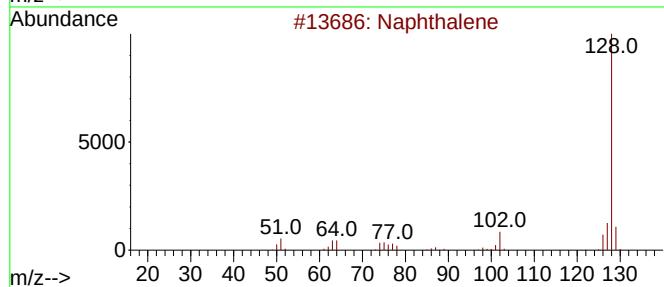
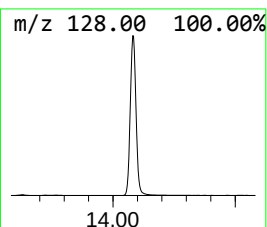
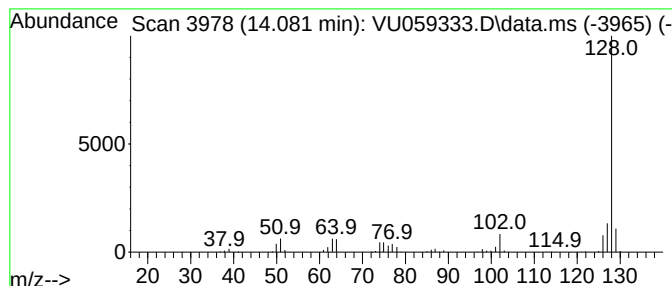
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Quant Title : VOC Analysis

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

Peak Number 5 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.081	121.77 ug/L	1025090	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			Naphthalene	128	C10H8	000091-20-3	91
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
Data File : VU059333.D
Acq On : 18 Jun 2024 23:48
Operator : MD/SY
Sample : P2873-09 200X
Misc : 3.28g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SJ9

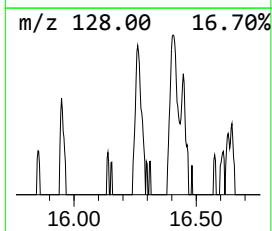
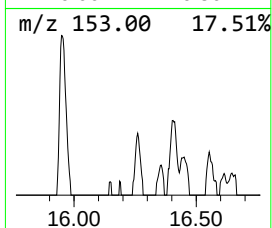
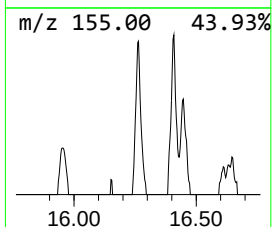
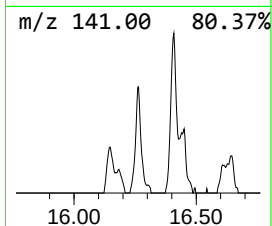
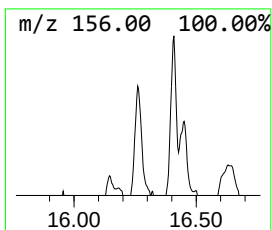
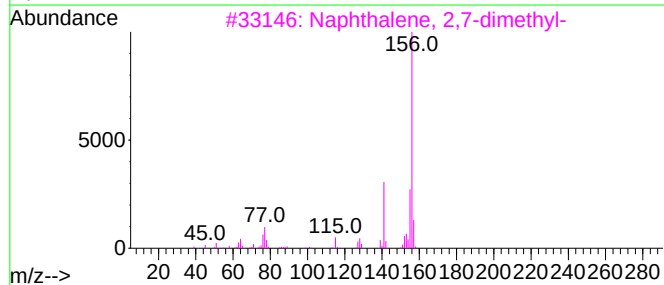
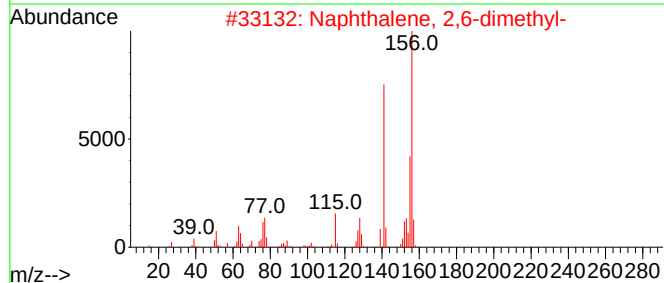
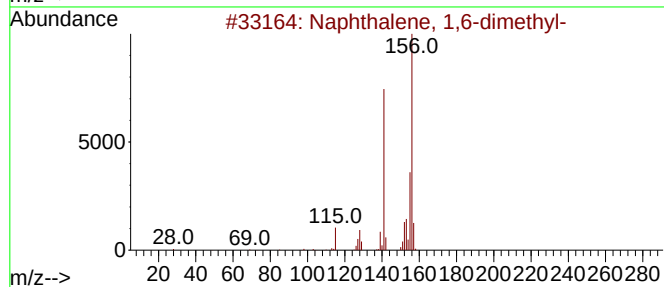
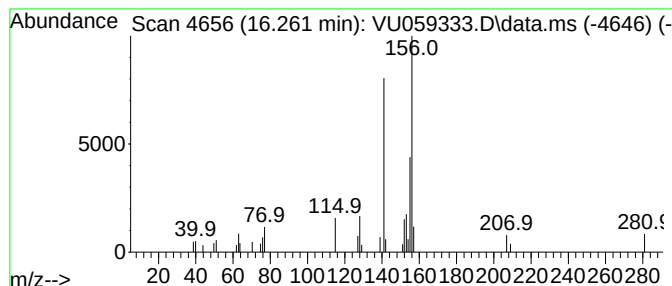
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Quant Title : VOC Analysis

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

Peak Number 8 Naphthalene, 1,6-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.261	2.59 ug/L	21792	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	93
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	93
3			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	91
4			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	90
5			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	87



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
Data File : VU059333.D
Acq On : 18 Jun 2024 23:48
Operator : MD/SY
Sample : P2873-09 200X
Misc : 3.28g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SJ9

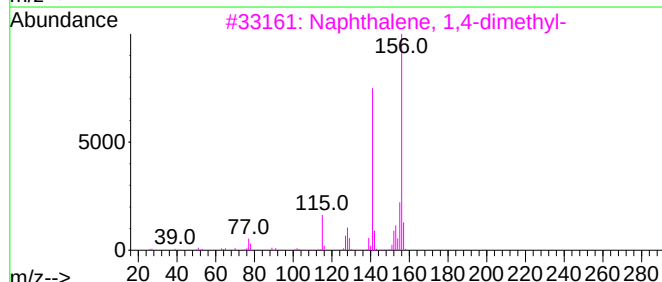
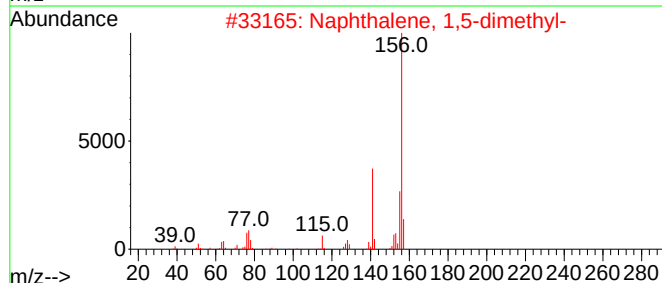
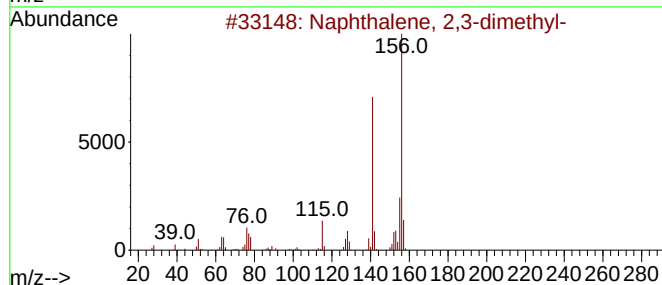
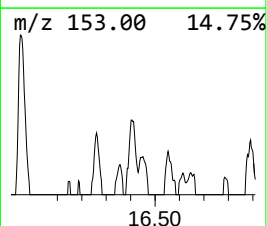
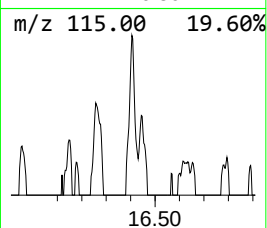
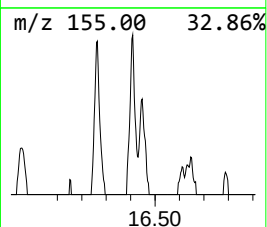
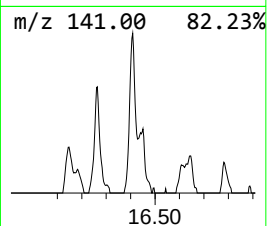
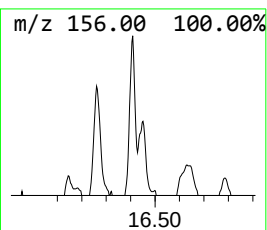
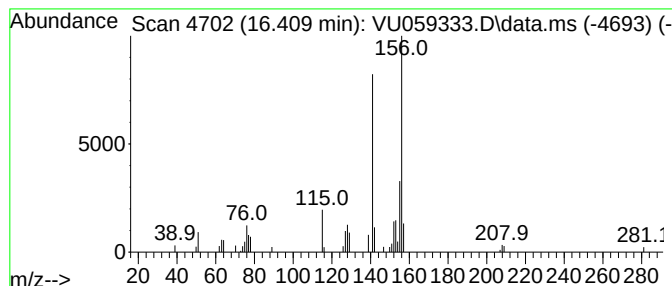
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Quant Title : VOC Analysis

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

Peak Number 9 Naphthalene, 2,3-dimethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.409	3.30 ug/L	27793	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, 1,5-dimethyl-	156	C12H12	000571-61-9	97
3			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	97
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	96
5			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
Data File : VU059333.D
Acq On : 18 Jun 2024 23:48
Operator : MD/SY
Sample : P2873-09 200X
Misc : 3.28g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0SJ9

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-ethe...	11.537	5.0	ug/L	42240	3	11.807	420903	50.0
Indene	12.309	6.2	ug/L	52190	3	11.807	420903	50.0
1H-Indene, 1-me...	13.627	2.7	ug/L	22431	3	11.807	420903	50.0
Azulene	14.081	121.8	ug/L	1025090	3	11.807	420903	50.0
Naphthalene, 1,...	16.261	2.6	ug/L	21792	3	11.807	420903	50.0
Naphthalene, 2,...	16.409	3.3	ug/L	27793	3	11.807	420903	50.0