

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
 Data File : VX025624.D
 Acq On : 08 Dec 2021 16:23
 Operator : JC/MD
 Sample : M4883-08ME
 Misc : 5.06g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW9G4ME

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_X\Method\SFAMXLM112221WMA.M
 Title : VOC Analysis

Signal : TIC: VX025624.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	23	26	31	rVB3	3456	5461	1.03%	0.116%
2	1.368	43	46	54	rVB	61393	69442	13.10%	1.475%
3	1.648	88	92	100	rBV	38000	46807	8.83%	0.994%
4	2.282	190	196	205	rBV	111800	182640	34.45%	3.879%
5	2.947	299	305	313	rBV3	2828	6820	1.29%	0.145%
6	4.489	550	558	584	rVB2	23777	105049	19.82%	2.231%
7	5.068	642	653	668	rVB	64432	199772	37.68%	4.243%
8	5.702	755	757	758	rBV	457	452	0.09%	0.010%
9	5.970	790	801	820	rBV2	182321	530111	100.00%	11.260%
10	6.367	860	866	867	rBV2	2015	3423	0.65%	0.073%
11	6.592	899	903	905	rBV2	437	737	0.14%	0.016%
12	6.763	922	931	948	rBV	124065	316447	59.69%	6.722%
13	7.129	982	991	1003	rBV	127367	282475	53.29%	6.000%
14	7.312	1013	1021	1041	rVB	99341	240184	45.31%	5.102%
15	7.470	1043	1047	1048	rBV	481	597	0.11%	0.013%
16	7.543	1058	1059	1061	rBV	347	323	0.06%	0.007%
17	7.568	1061	1063	1066	rVB	383	364	0.07%	0.008%
18	7.598	1066	1068	1070	rBV	333	353	0.07%	0.007%
19	7.958	1123	1127	1129	rBV3	593	796	0.15%	0.017%
20	8.183	1162	1164	1169	rVB2	466	520	0.10%	0.011%
21	8.330	1182	1188	1200	rVB	60530	107175	20.22%	2.276%
22	8.476	1210	1212	1214	rBV2	310	347	0.07%	0.007%
23	8.604	1229	1233	1234	rBV2	832	1259	0.24%	0.027%
24	8.653	1234	1241	1248	rVV	266920	439860	82.98%	9.343%
25	8.720	1249	1252	1258	rVB	6633	10503	1.98%	0.223%
26	8.909	1281	1283	1285	rBV3	857	914	0.17%	0.019%
27	8.958	1285	1291	1301	rVB	39641	67794	12.79%	1.440%
28	9.098	1312	1314	1317	rVB2	411	455	0.09%	0.010%
29	9.159	1321	1324	1327	rBV2	337	536	0.10%	0.011%
30	9.275	1338	1343	1349	rVV2	8347	12401	2.34%	0.263%
31	9.397	1357	1363	1376	rBV	148071	236824	44.67%	5.030%
32	9.561	1388	1390	1392	rVB2	796	516	0.10%	0.011%
33	9.616	1395	1399	1405	rVB3	1007	1676	0.32%	0.036%
34	9.708	1412	1414	1418	rVB2	839	1168	0.22%	0.025%
35	9.817	1429	1432	1437	rVB2	726	1051	0.20%	0.022%
36	9.903	1445	1446	1450	rVB	767	687	0.13%	0.015%

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Instrument :
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 ClientSampleId :
 EW9G4ME

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 >

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
 Title : VOC Analysis

37	10.006	1461	1463	1466	rVV3	496	581	0.11%	0.012%
38	10.061	1466	1472	1480	rVV	252345	373950	70.54%	7.943%
39	10.195	1490	1494	1498	rBV	902	1218	0.23%	0.026%
40	10.305	1507	1512	1517	rVV3	4984	7646	1.44%	0.162%
41	10.360	1517	1521	1525	rVB2	1593	2227	0.42%	0.047%
42	10.451	1535	1536	1538	rBV	444	437	0.08%	0.009%
43	10.555	1549	1553	1554	rVV	442	423	0.08%	0.009%
44	10.585	1556	1558	1561	rVV2	763	786	0.15%	0.017%
45	10.646	1564	1568	1575	rVB4	2518	4324	0.82%	0.092%
46	10.774	1583	1589	1593	rVV3	838	1853	0.35%	0.039%
47	10.860	1600	1603	1605	rBV2	634	716	0.14%	0.015%
48	10.896	1605	1609	1612	rVV3	726	1200	0.23%	0.025%
49	11.085	1638	1640	1642	rBV2	584	545	0.10%	0.012%
50	11.122	1642	1646	1649	rVB4	3218	4111	0.78%	0.087%
51	11.195	1653	1658	1666	rBV	183027	246174	46.44%	5.229%
52	11.274	1669	1671	1674	rBV2	514	560	0.11%	0.012%
53	11.384	1686	1689	1697	rVB2	744	1350	0.25%	0.029%
54	11.463	1697	1702	1703	rBV2	2099	3107	0.59%	0.066%
55	11.543	1714	1715	1718	rVB2	459	497	0.09%	0.011%
56	11.622	1723	1728	1729	rBV2	622	979	0.18%	0.021%
57	11.713	1741	1743	1746	rBV2	1232	1439	0.27%	0.031%
58	11.756	1746	1750	1756	rVB2	4871	6994	1.32%	0.149%
59	11.811	1756	1759	1762	rBV2	744	821	0.15%	0.017%
60	11.847	1762	1765	1768	rBB2	643	770	0.15%	0.016%
61	11.939	1776	1780	1783	rBV3	1809	2571	0.48%	0.055%
62	12.024	1789	1794	1800	rBV	318768	388294	73.25%	8.248%
63	12.152	1812	1815	1818	rVB3	2302	2456	0.46%	0.052%
64	12.225	1824	1827	1830	rBV3	1080	1575	0.30%	0.033%
65	12.323	1837	1843	1851	rVB	333279	410311	77.40%	8.715%
66	12.384	1851	1853	1855	rVV2	701	743	0.14%	0.016%
67	12.427	1856	1860	1864	rVV3	4784	5731	1.08%	0.122%
68	12.481	1865	1869	1874	rVB7	1231	2256	0.43%	0.048%
69	12.890	1934	1936	1939	rBV4	947	1165	0.22%	0.025%
70	12.975	1945	1950	1954	rVB4	1947	3246	0.61%	0.069%
71	13.048	1958	1962	1966	rVB3	966	1635	0.31%	0.035%
72	13.207	1986	1988	1989	rBV	804	527	0.10%	0.011%
73	13.237	1991	1993	1994	rVV	665	482	0.09%	0.010%
74	13.268	1995	1998	2009	rVB4	4260	6534	1.23%	0.139%
75	13.341	2009	2010	2013	rBV	359	402	0.08%	0.009%
76	13.390	2013	2018	2022	rBV2	2108	2897	0.55%	0.062%

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Instrument :
 MSVOA_X
 ClientSampleId :
 EW9G4ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML112221WMA.M
 Title : VOC Analysis

77	13.500	2033	2036	2038	rBV2	492	418	0.08%	0.009%
78	13.585	2048	2050	2051	rBV	462	375	0.07%	0.008%
79	13.676	2063	2065	2066	rBV	752	732	0.14%	0.016%
80	13.780	2077	2082	2089	rVB	97979	122772	23.16%	2.608%
81	13.847	2089	2093	2096	rBV2	2915	3715	0.70%	0.079%
82	13.926	2104	2106	2110	rVB2	780	904	0.17%	0.019%
83	13.957	2110	2111	2113	rBV	540	438	0.08%	0.009%
84	13.999	2114	2118	2119	rVV3	723	1041	0.20%	0.022%
85	14.042	2122	2125	2129	rVB3	4935	5763	1.09%	0.122%
86	14.316	2168	2170	2172	rVB3	582	477	0.09%	0.010%
87	14.420	2185	2187	2188	rBV2	808	502	0.09%	0.011%
88	14.475	2194	2196	2197	rBV2	677	516	0.10%	0.011%
89	14.566	2208	2211	2215	rBV5	1311	1902	0.36%	0.040%
90	14.640	2216	2223	2231	rVB	38882	49972	9.43%	1.061%
91	14.780	2236	2246	2253	rBV	28688	47134	8.89%	1.001%
92	15.213	2314	2317	2322	rVB3	5711	6663	1.26%	0.142%
93	15.481	2356	2361	2367	rBV	12979	20686	3.90%	0.439%
94	15.615	2378	2383	2387	rBV2	22912	37859	7.14%	0.804%
95	15.816	2411	2416	2418	rBV3	5854	10083	1.90%	0.214%
96	16.097	2458	2462	2468	rVB2	4266	7169	1.35%	0.152%
97	16.200	2476	2479	2485	rVB3	1229	1804	0.34%	0.038%
98	16.334	2497	2501	2512	rVB5	3783	9292	1.75%	0.197%
99	16.548	2534	2536	2537	rBV	895	589	0.11%	0.013%
100	16.664	2550	2555	2558	rBV3	4506	7687	1.45%	0.163%

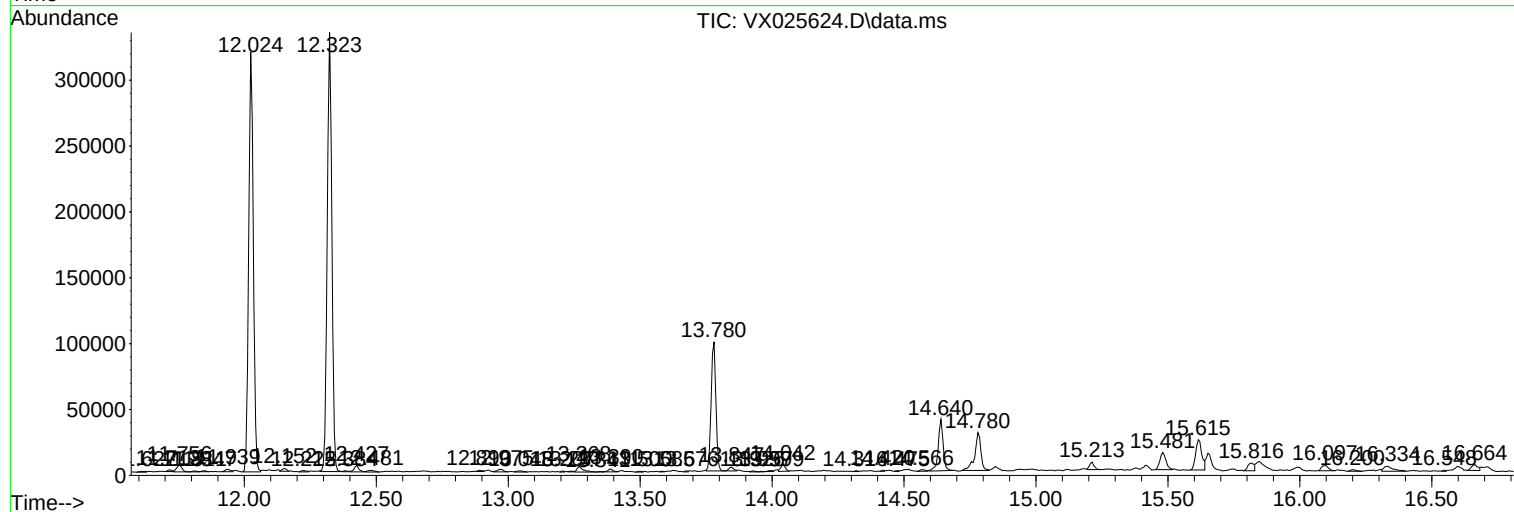
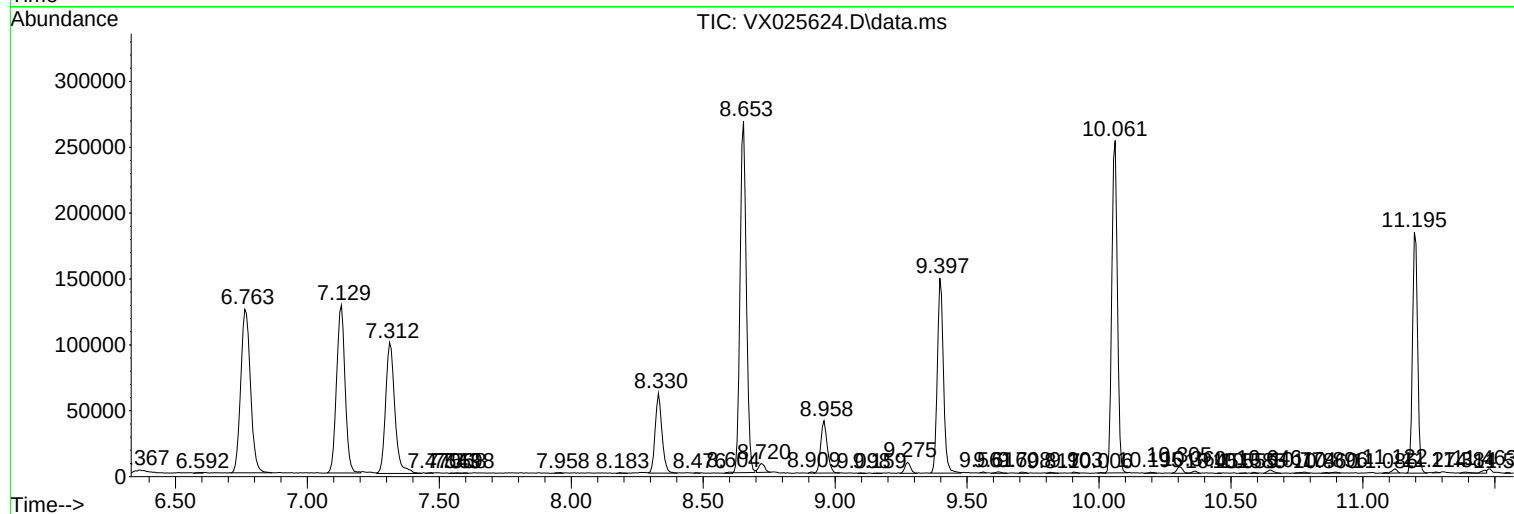
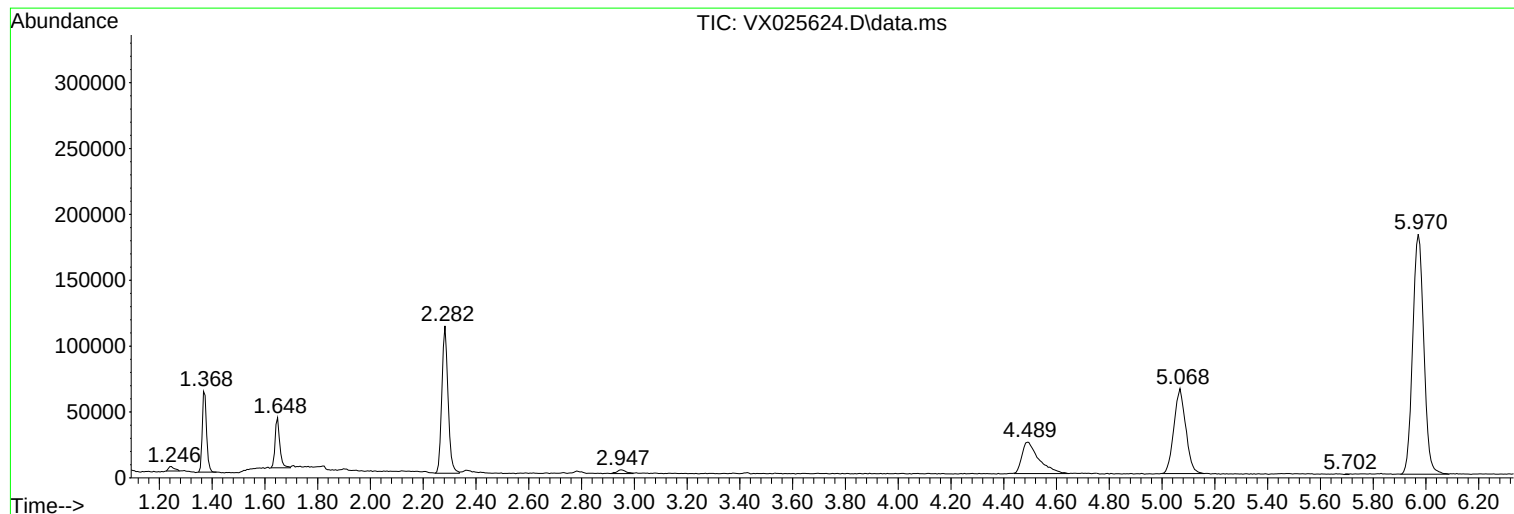
Sum of corrected areas: 4707965

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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9G4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9G4ME

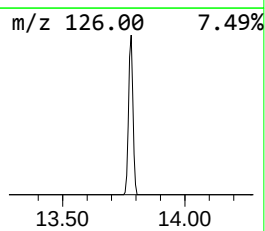
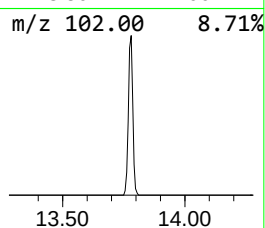
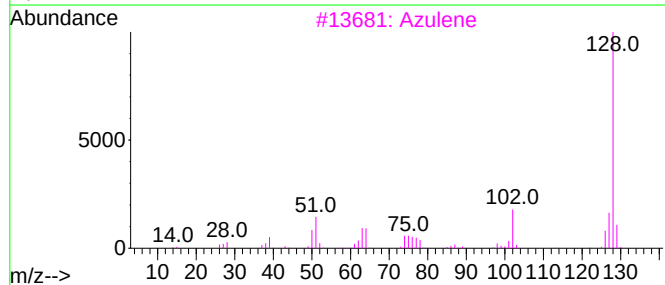
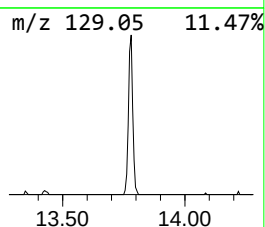
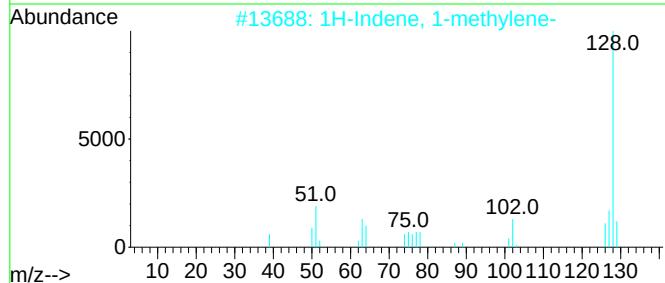
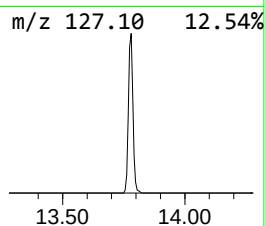
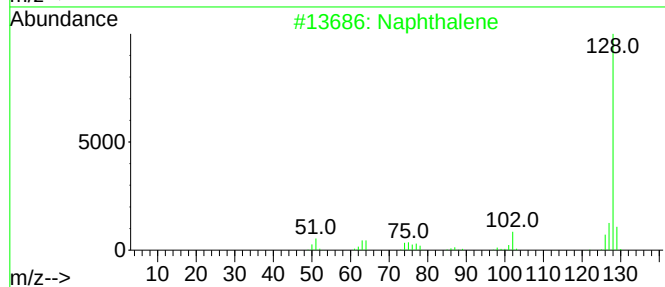
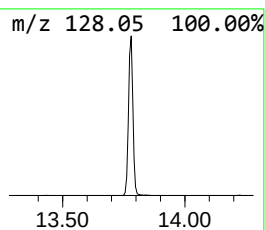
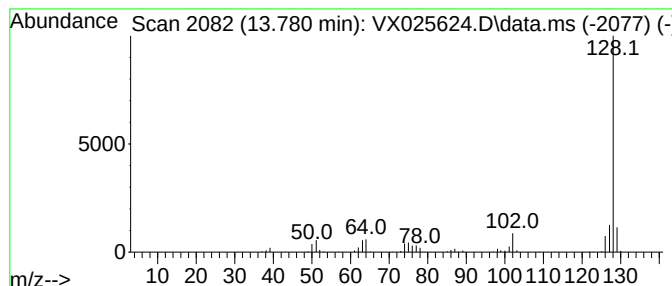
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	15.81 ug/L	122772	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	91
3			Azulene	128	C10H8	000275-51-4	91
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	90



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Instrument :
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ClientSampleId :
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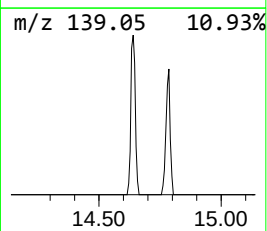
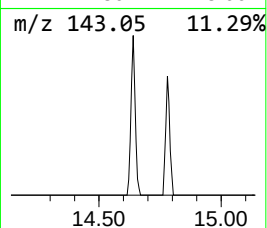
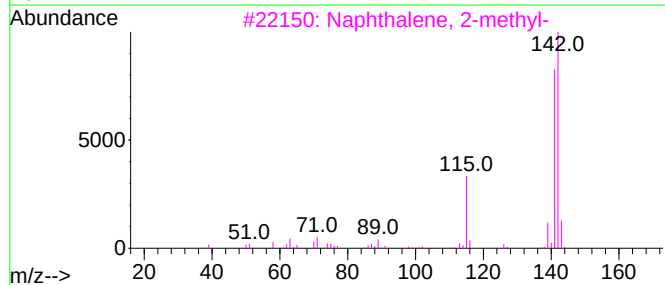
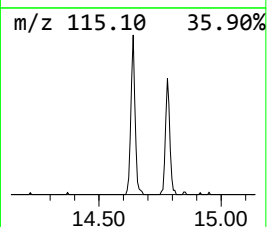
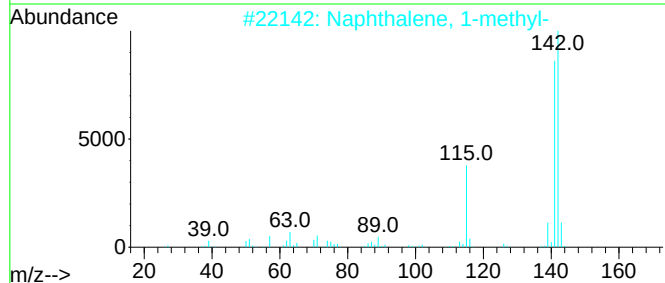
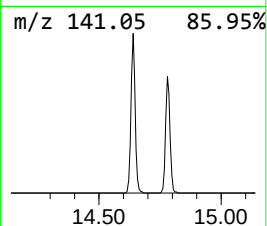
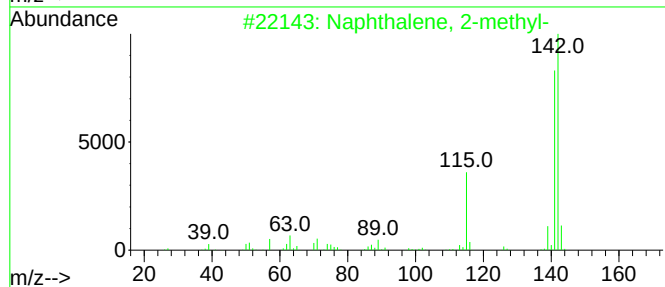
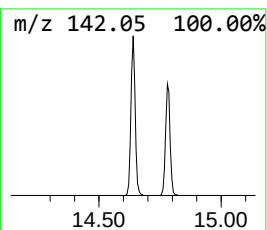
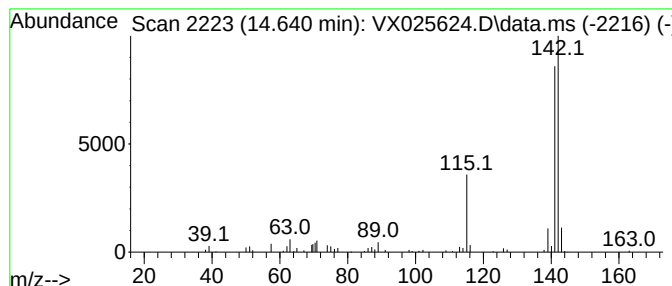
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Naphthalene, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	6.43 ug/L	49972	1,4-Dichlorobenzene-d4	12.024

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



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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9G4ME

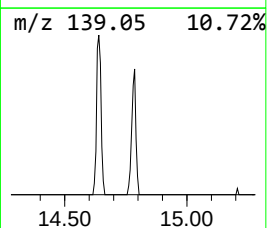
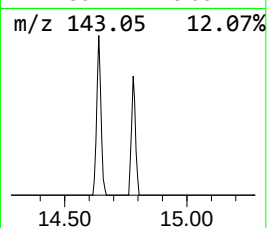
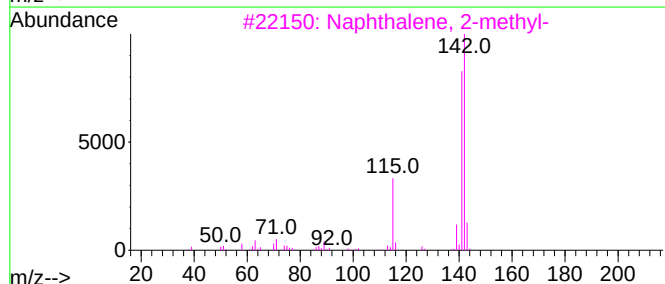
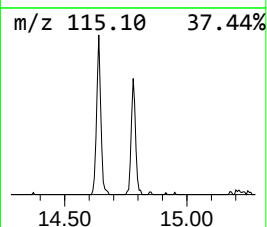
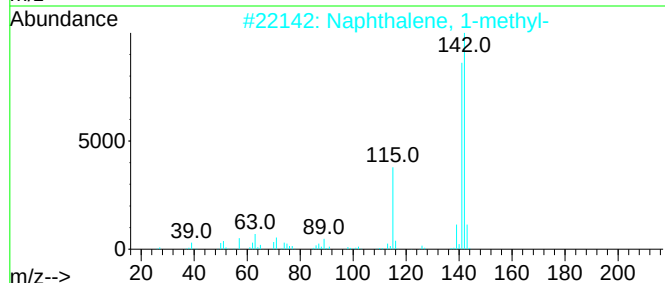
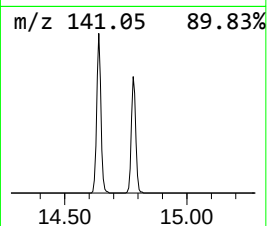
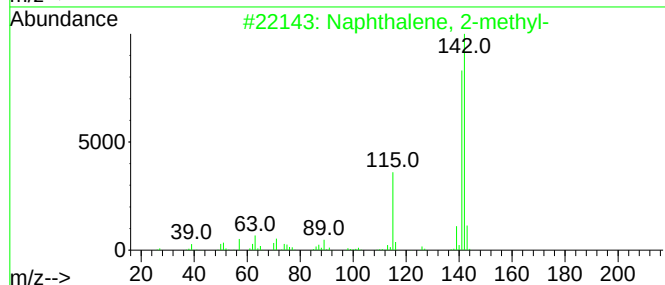
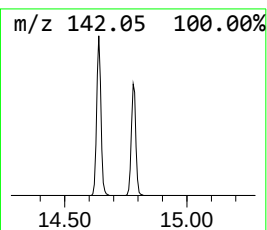
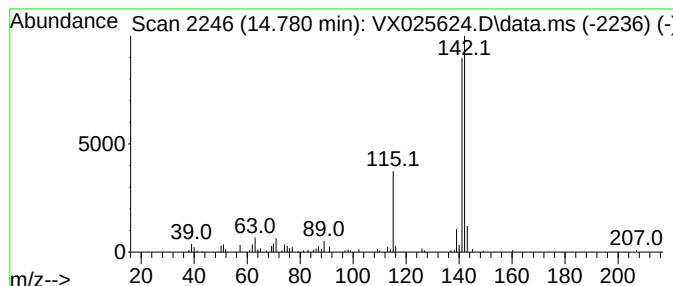
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Naphthalene, 1-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	6.07 ug/L	47134	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
4			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
5			Benzocycloheptatriene	142	C11H10	000264-09-5	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025624.D
Acq On : 08 Dec 2021 16:23
Operator : JC/MD
Sample : M4883-08ME
Misc : 5.06g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9G4ME

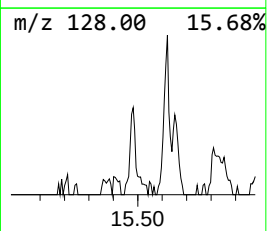
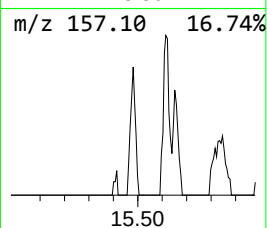
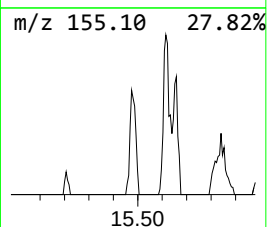
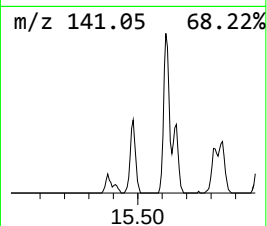
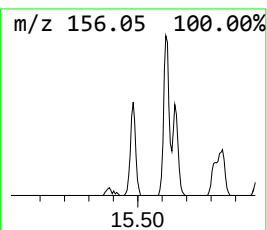
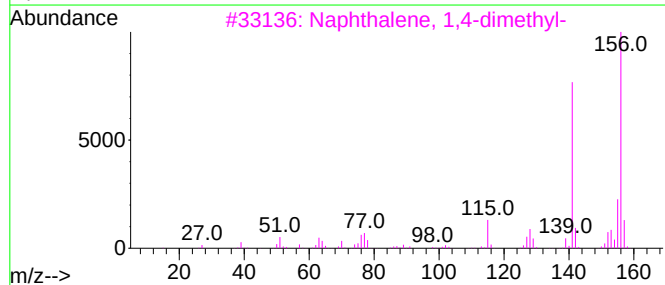
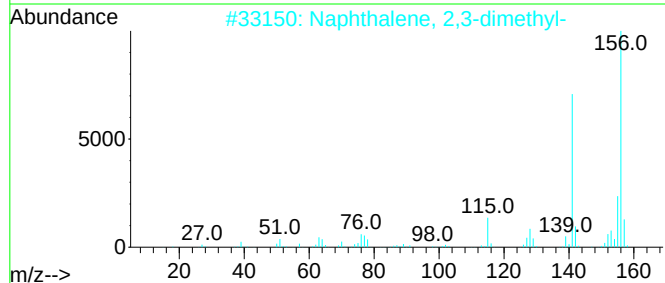
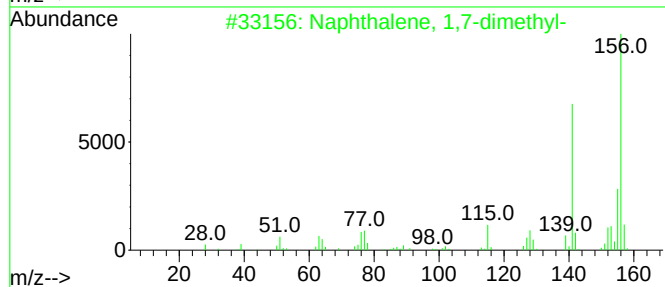
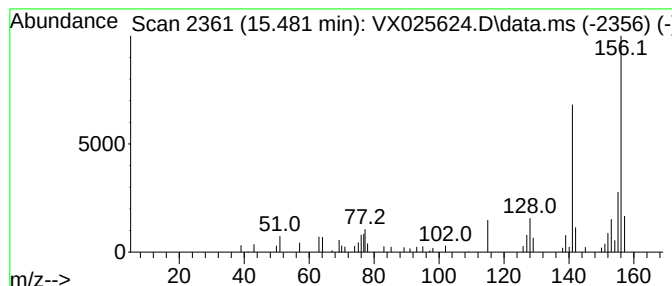
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Quant Title : VOC Analysis

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

Peak Number 5 Naphthalene, 1,7-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.481	2.66 ug/L	20686	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
2			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
3			Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	96
4			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	96
5			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025624.D
Acq On : 08 Dec 2021 16:23
Operator : JC/MD
Sample : M4883-08ME
Misc : 5.06g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9G4ME

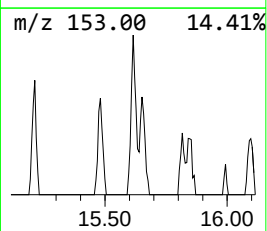
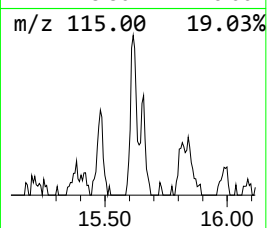
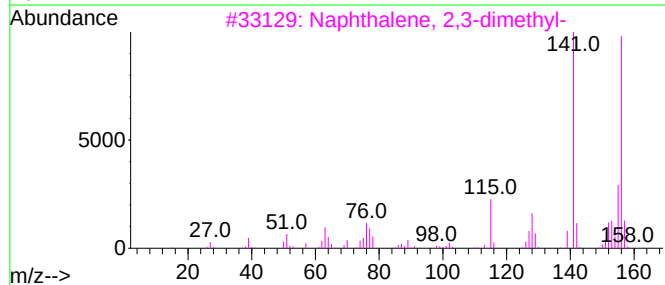
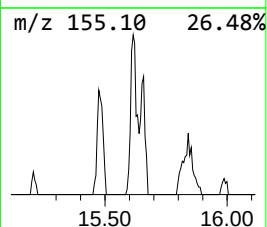
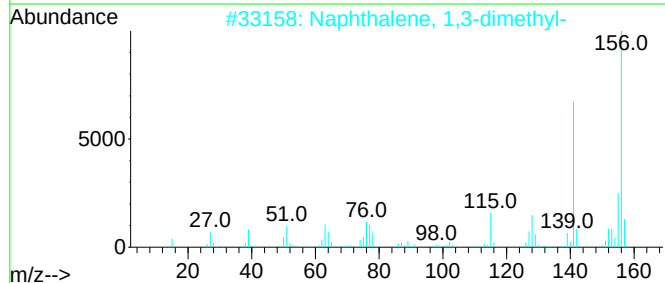
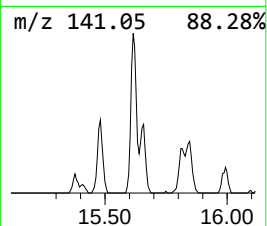
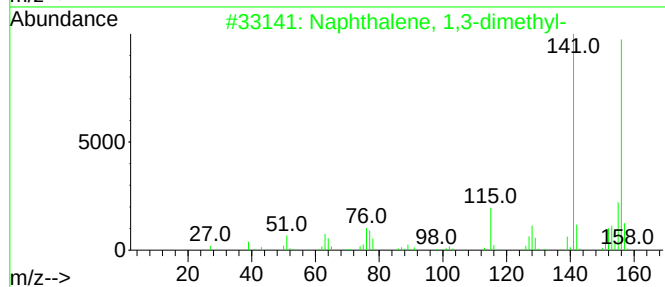
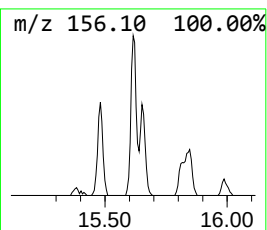
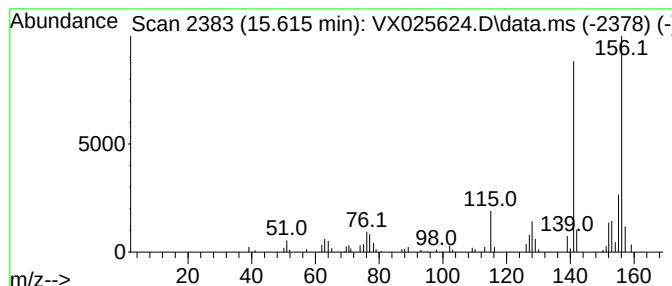
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Quant Title : VOC Analysis

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

Peak Number 6 Naphthalene, 1,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	4.88 ug/L	37859	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	98
2			Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	97
3			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
4			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	97
5			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025624.D
Acq On : 08 Dec 2021 16:23
Operator : JC/MD
Sample : M4883-08ME
Misc : 5.06g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9G4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML112221WMA.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
Azulene	13.780	15.8	ug/L	122772	3	12.024	388294	50.0
Naphthalene, 2-...	14.640	6.4	ug/L	49972	3	12.024	388294	50.0
Naphthalene, 1-...	14.780	6.1	ug/L	47134	3	12.024	388294	50.0
Naphthalene, 1,...	15.481	2.7	ug/L	20686	3	12.024	388294	50.0
Naphthalene, 1,...	15.615	4.9	ug/L	37859	3	12.024	388294	50.0