

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
 Data File : VX042772.D
 Acq On : 31 Jul 2024 14:50
 Operator : JC/MD
 Sample : P3348-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VHBLK001

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\SFAMXML072624WMA.M
 Title : VOC Analysis

Signal : TIC: VX042772.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	22	25	35	rBV	15334	20753	4.85%	0.559%
2	1.367	43	46	58	rVB	29734	39805	9.31%	1.072%
3	1.648	89	92	102	rVB	28636	36173	8.46%	0.975%
4	2.233	185	188	190	rBV	135	199	0.05%	0.005%
5	2.294	192	198	211	rVV	82266	128042	29.95%	3.450%
6	2.514	231	234	236	rBB	218	191	0.04%	0.005%
7	2.556	240	241	245	rVB	187	181	0.04%	0.005%
8	2.642	252	255	256	rBV	194	191	0.04%	0.005%
9	2.697	262	264	269	rBV	171	286	0.07%	0.008%
10	2.788	275	279	286	rBV6	1163	2684	0.63%	0.072%
11	2.946	300	305	314	rVV2	4813	10798	2.53%	0.291%
12	3.178	341	343	346	rBB	141	150	0.04%	0.004%
13	3.288	358	361	365	rBV	183	240	0.06%	0.006%
14	3.562	404	406	407	rVV	289	176	0.04%	0.005%
15	4.074	487	490	491	rVB	202	155	0.04%	0.004%
16	4.105	492	495	498	rBB	177	157	0.04%	0.004%
17	4.196	507	510	513	rBV	302	358	0.08%	0.010%
18	4.227	513	515	518	rVB2	256	245	0.06%	0.007%
19	4.471	547	555	569	rBV	28382	82166	19.22%	2.214%
20	4.830	610	614	616	rBB	217	259	0.06%	0.007%
21	4.891	621	624	625	rBV	173	182	0.04%	0.005%
22	5.056	638	651	667	rBV2	54621	170336	39.84%	4.589%
23	5.196	672	674	676	rVV2	286	196	0.05%	0.005%
24	5.245	680	682	684	rVB2	178	154	0.04%	0.004%
25	5.312	690	693	695	rBB2	162	140	0.03%	0.004%
26	5.379	702	704	705	rBV	219	161	0.04%	0.004%
27	5.562	731	734	736	rBV	337	320	0.07%	0.009%
28	5.617	741	743	749	rBB	170	221	0.05%	0.006%
29	5.745	761	764	765	rBB	147	151	0.04%	0.004%
30	5.769	766	768	771	rBB	161	207	0.05%	0.006%
31	5.970	789	801	822	rBV3	147415	427536	100.00%	11.518%
32	6.257	845	848	850	rBV	161	146	0.03%	0.004%
33	6.348	860	863	865	rBB	179	212	0.05%	0.006%
34	6.617	906	907	909	rBV	186	143	0.03%	0.004%
35	6.763	922	931	944	rBV	120615	290628	67.98%	7.830%
36	6.988	965	968	969	rBV	204	169	0.04%	0.005%

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Integration Parameters: LSCINT.P

Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
 Title : VOC Analysis

37	7.123	985	990	996	rVB5	984	1760	0.41%	0.047%
38	7.312	1012	1021	1034	rBV	85529	192230	44.96%	5.179%
39	7.476	1044	1048	1051	rBV	247	361	0.08%	0.010%
40	7.531	1054	1057	1060	rBB	194	270	0.06%	0.007%
41	7.592	1064	1067	1070	rBB	223	308	0.07%	0.008%
42	7.659	1076	1078	1080	rBB	197	179	0.04%	0.005%
43	7.805	1100	1102	1104	rBB	226	188	0.04%	0.005%
44	7.879	1111	1114	1116	rBV	173	187	0.04%	0.005%
45	7.982	1129	1131	1133	rBV	191	147	0.03%	0.004%
46	8.037	1135	1140	1145	rBV2	182	436	0.10%	0.012%
47	8.122	1151	1154	1155	rBV2	172	152	0.04%	0.004%
48	8.165	1159	1161	1164	rBB	284	225	0.05%	0.006%
49	8.196	1164	1166	1168	rBV2	186	201	0.05%	0.005%
50	8.330	1181	1188	1201	rBV	51640	91149	21.32%	2.456%
51	8.543	1222	1223	1225	rBV	206	151	0.04%	0.004%
52	8.647	1234	1240	1251	rBV	220045	355864	83.24%	9.587%
53	8.872	1273	1277	1283	rBB	289	545	0.13%	0.015%
54	8.951	1285	1290	1302	rBV	39358	59878	14.01%	1.613%
55	9.086	1311	1312	1316	rBB	158	173	0.04%	0.005%
56	9.116	1316	1317	1319	rBV	214	163	0.04%	0.004%
57	9.165	1323	1325	1327	rBV	174	151	0.04%	0.004%
58	9.281	1341	1344	1345	rBV	196	159	0.04%	0.004%
59	9.384	1356	1361	1379	rBV	127359	202039	47.26%	5.443%
60	9.634	1401	1402	1405	rBV	184	203	0.05%	0.005%
61	9.701	1407	1413	1418	rBV3	1062	1783	0.42%	0.048%
62	9.939	1450	1452	1455	rVB3	191	205	0.05%	0.006%
63	10.055	1465	1471	1483	rBV	246237	343686	80.39%	9.259%
64	10.305	1509	1512	1513	rBV	500	482	0.11%	0.013%
65	10.549	1551	1552	1556	rVB	184	147	0.03%	0.004%
66	10.616	1561	1563	1565	rBV	211	173	0.04%	0.005%
67	10.646	1565	1568	1570	rVB	287	334	0.08%	0.009%
68	10.701	1571	1577	1578	rBB	199	241	0.06%	0.006%
69	10.787	1589	1591	1592	rVB	314	157	0.04%	0.004%
70	10.817	1593	1596	1599	rBB	214	244	0.06%	0.007%
71	10.847	1599	1601	1607	rBB	286	427	0.10%	0.012%
72	10.896	1607	1609	1611	rBB	157	162	0.04%	0.004%
73	10.963	1616	1620	1624	rBV	407	606	0.14%	0.016%
74	11.036	1629	1632	1634	rBV	235	249	0.06%	0.007%
75	11.104	1641	1643	1648	rVB	167	236	0.06%	0.006%
76	11.146	1648	1650	1652	rBV	138	148	0.03%	0.004%

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 ClientSampleId :
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 Title : VOC Analysis

77	11.189	1652	1657	1665	rBV	173692	236936	55.42%	6.383%
78	11.372	1686	1687	1690	rBB	205	165	0.04%	0.004%
79	11.402	1690	1692	1695	rBV	258	323	0.08%	0.009%
80	11.591	1719	1723	1725	rBV2	242	304	0.07%	0.008%
81	11.689	1737	1739	1742	rBB	177	147	0.03%	0.004%
82	11.756	1745	1750	1756	rBV2	463	867	0.20%	0.023%
83	12.024	1789	1794	1804	rBV	267944	346717	81.10%	9.341%
84	12.213	1823	1825	1826	rBV	381	302	0.07%	0.008%
85	12.244	1827	1830	1837	rVB2	4168	4845	1.13%	0.131%
86	12.323	1837	1843	1851	rBV	259332	350466	81.97%	9.442%
87	13.073	1965	1966	1969	rBV3	412	520	0.12%	0.014%
88	13.640	2057	2059	2061	rBV	241	168	0.04%	0.005%
89	13.774	2076	2081	2090	rBV	102295	135564	31.71%	3.652%
90	13.957	2109	2111	2115	rBV3	305	291	0.07%	0.008%
91	14.066	2128	2129	2134	rBV2	306	425	0.10%	0.011%
92	14.127	2134	2139	2146	rVB2	3642	6043	1.41%	0.163%
93	14.182	2146	2148	2150	rBV2	553	665	0.16%	0.018%
94	14.353	2174	2176	2178	rBV	473	283	0.07%	0.008%
95	14.639	2219	2223	2228	rVB	12081	15555	3.64%	0.419%
96	14.780	2241	2246	2254	rBV2	22348	27988	6.55%	0.754%
97	15.206	2312	2316	2322	rVB	5804	8972	2.10%	0.242%
98	16.090	2457	2461	2466	rBV3	2121	3555	0.83%	0.096%
99	16.328	2493	2500	2506	rBV2	33943	61589	14.41%	1.659%
100	16.688	2553	2559	2569	rBV2	18460	38669	9.04%	1.042%

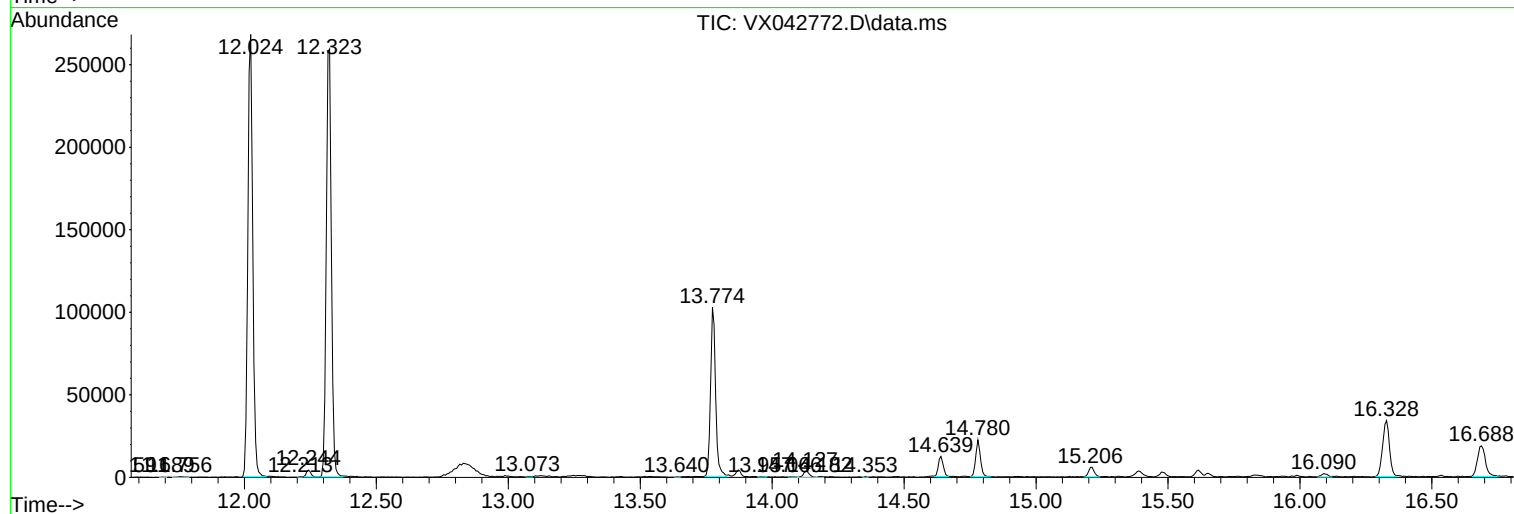
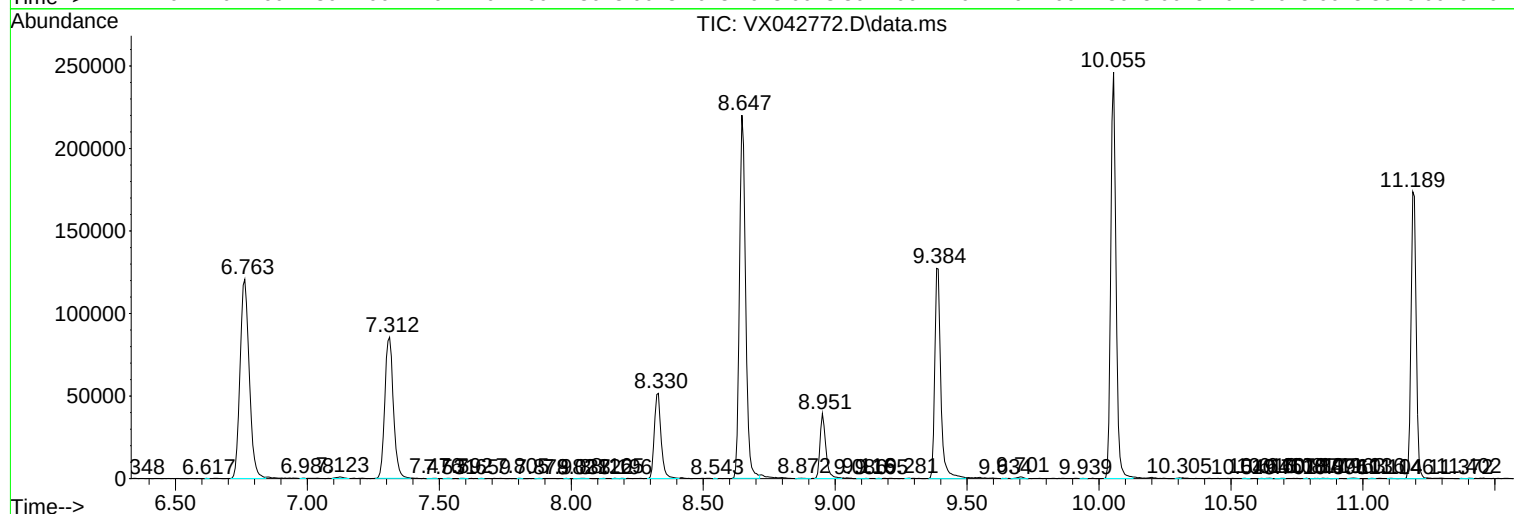
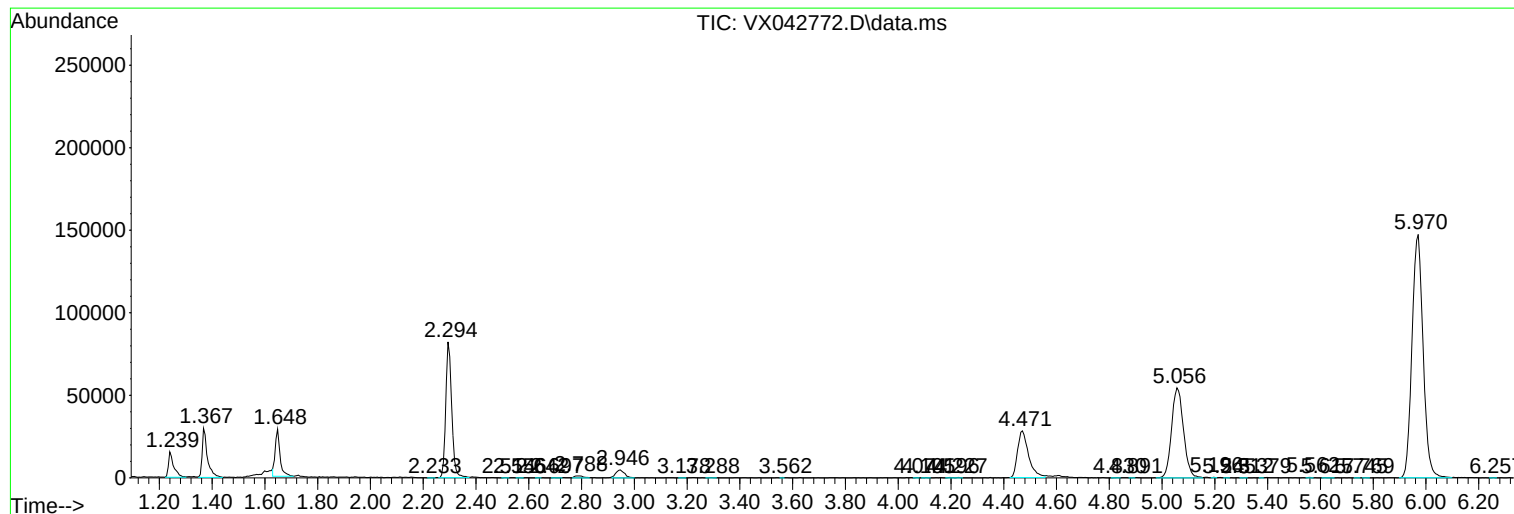
Sum of corrected areas: 3711869

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ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VHBLK001

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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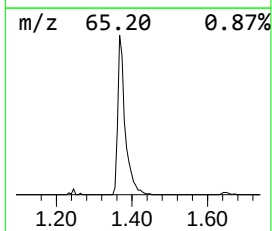
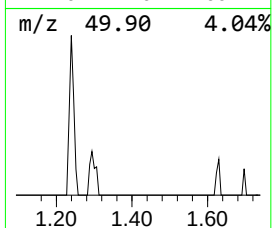
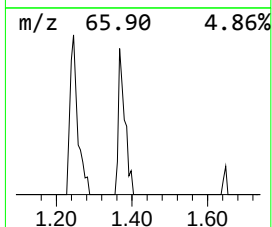
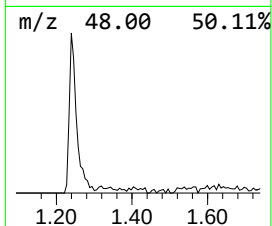
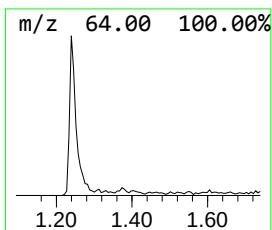
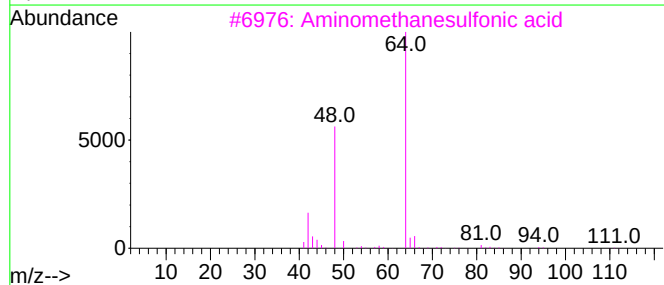
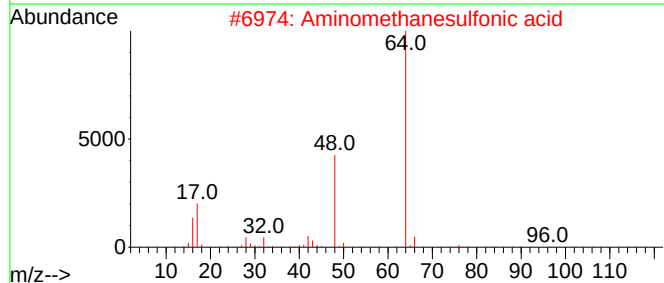
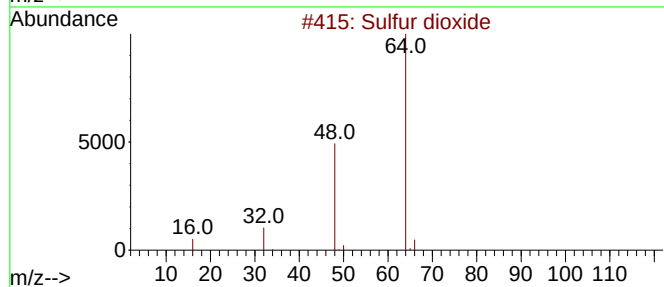
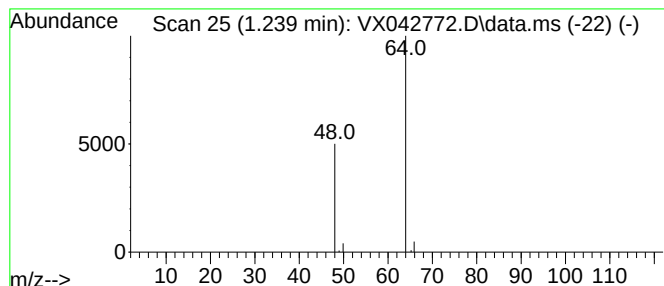
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.239	3.57 ug/L	20753	1,4-Difluorobenzene	6.763

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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



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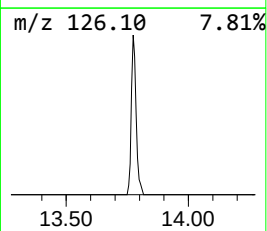
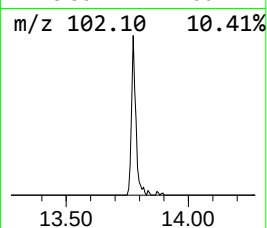
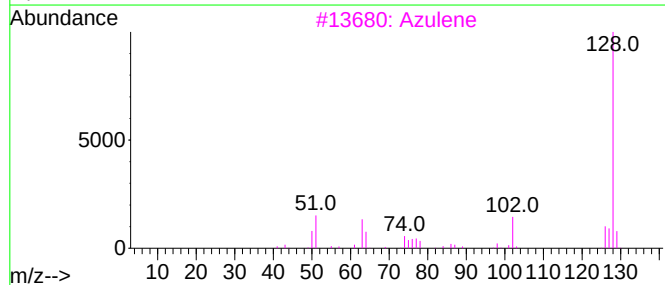
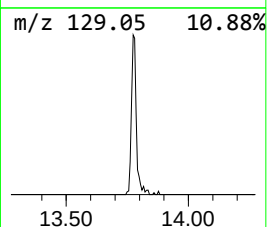
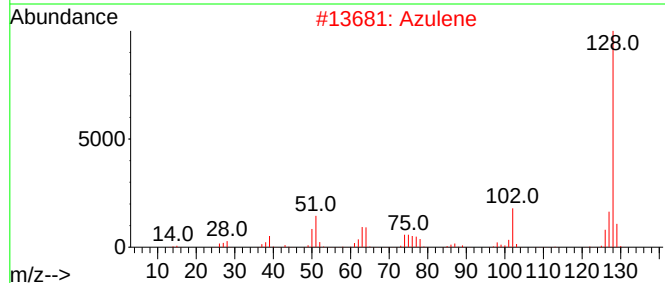
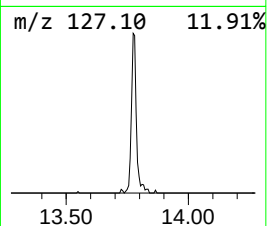
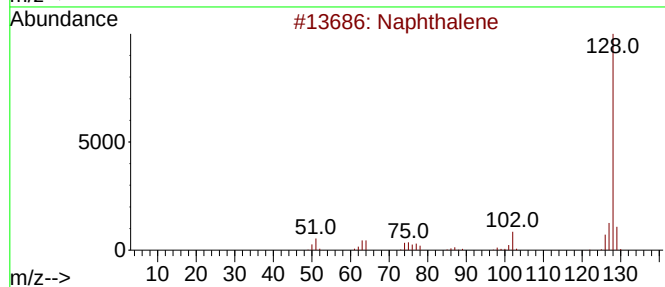
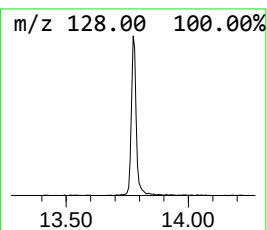
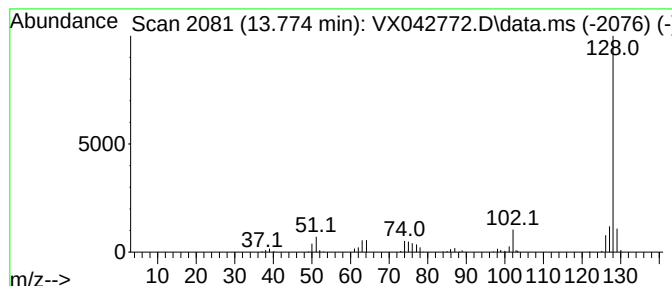
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM072624WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Azulene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	19.55 ug/L	135564	1,4-Dichlorobenzene-d4	12.024

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



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ClientSampleId :
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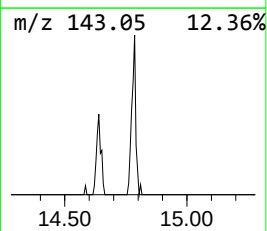
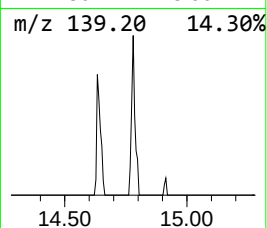
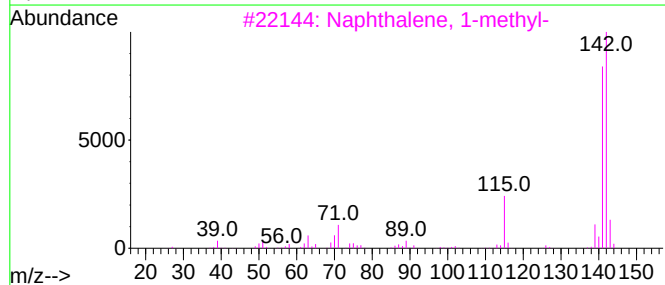
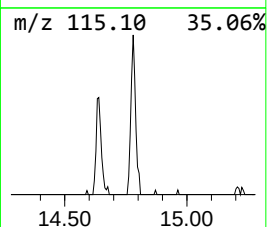
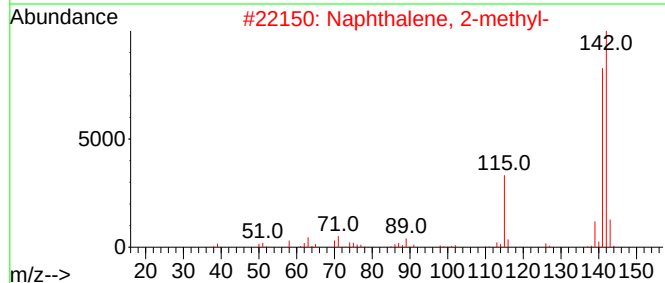
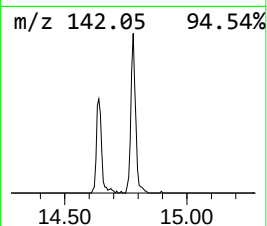
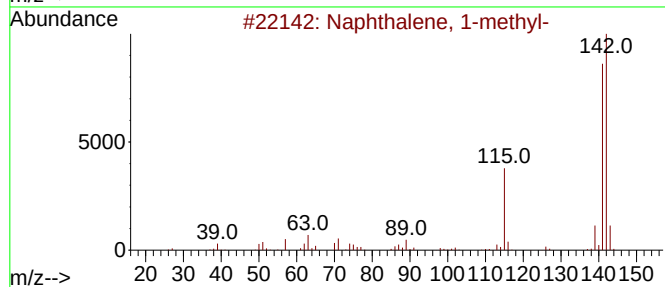
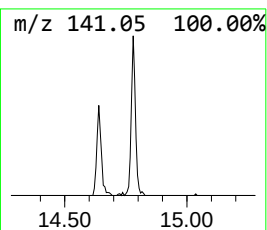
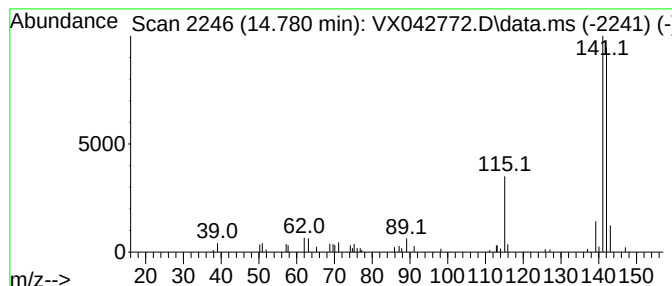
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Naphthalene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	4.04 ug/L	27988	1,4-Dichlorobenzene-d4	12.024

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
2		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	93
3		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
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\VX073124\
Data File : VX042772.D
Acq On : 31 Jul 2024 14:50
Operator : JC/MD
Sample : P3348-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VHBLK001

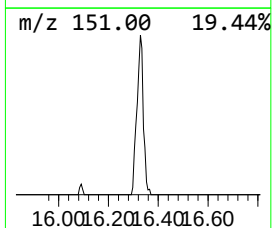
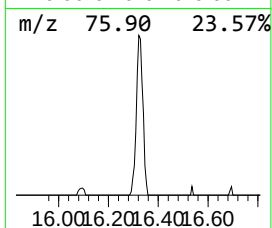
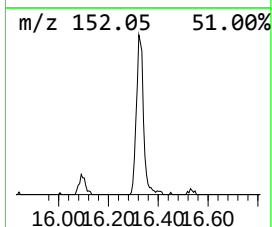
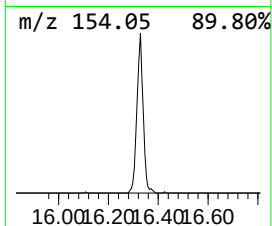
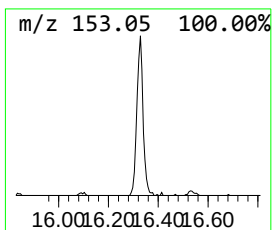
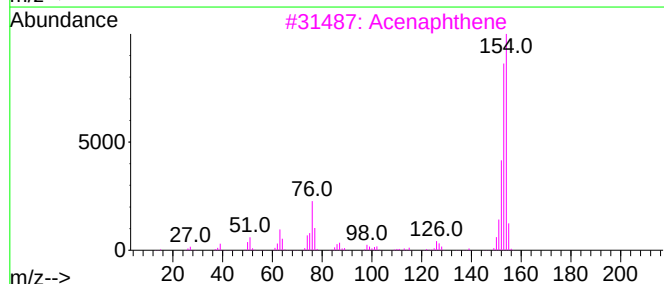
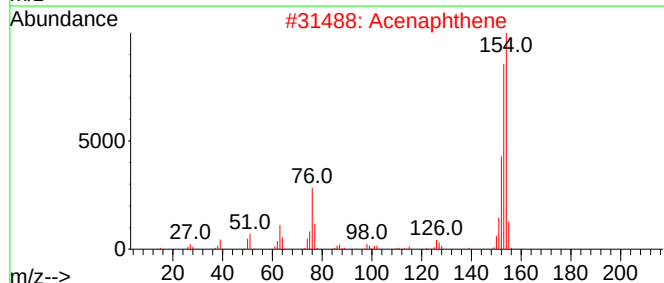
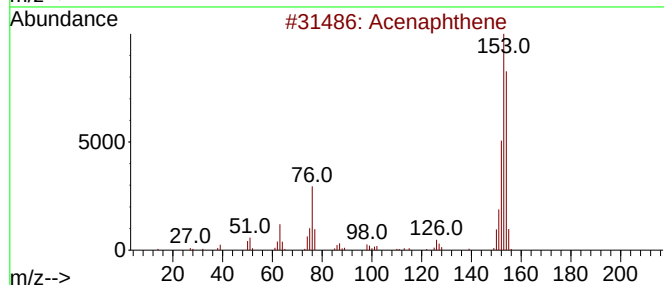
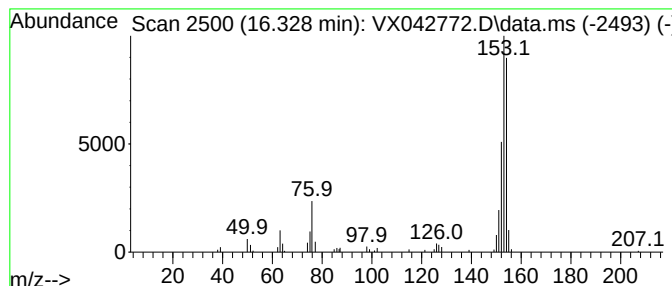
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Quant Title : VOC Analysis

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

Peak Number 5 Acenaphthene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.328	8.88 ug/L	61589	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	89
2			Acenaphthene	154	C12H10	000083-32-9	64
3			Acenaphthene	154	C12H10	000083-32-9	64
4			1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	59
5			Hexa-2,4-diyn-1-ylbenzene	154	C12H10	000520-74-1	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042772.D
Acq On : 31 Jul 2024 14:50
Operator : JC/MD
Sample : P3348-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VHBLK001

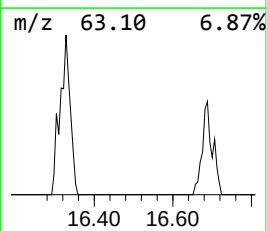
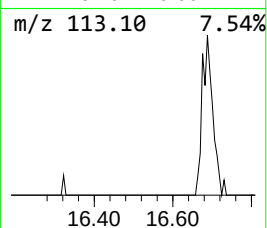
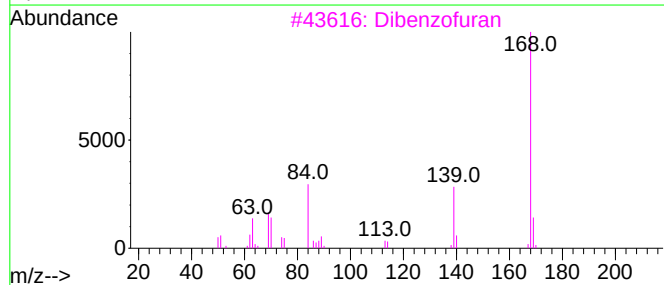
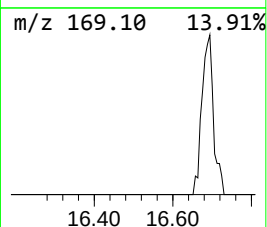
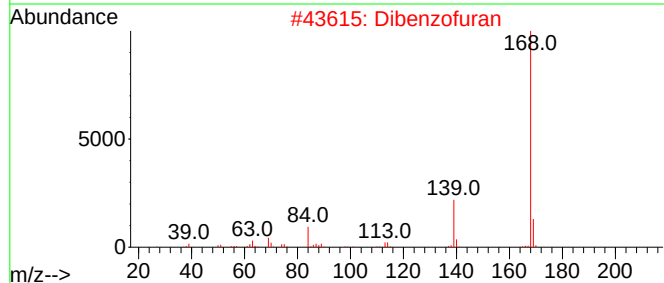
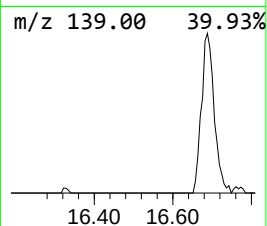
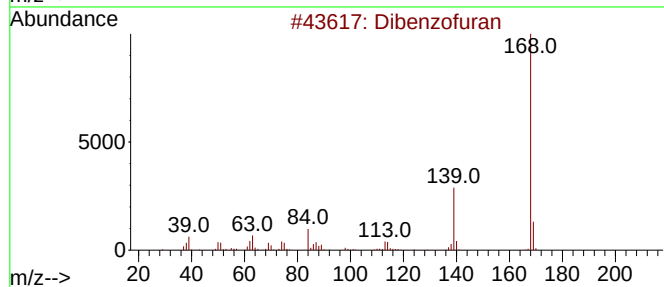
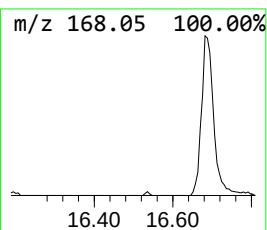
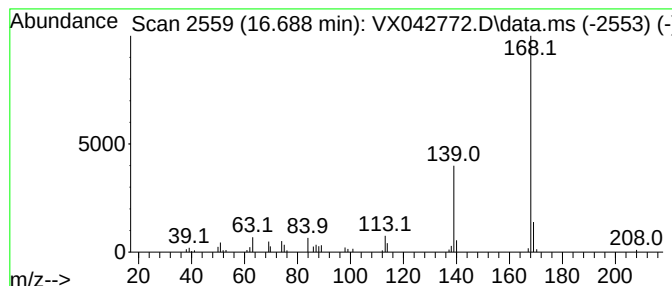
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Quant Title : VOC Analysis

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

Peak Number 6 Dibenzofuran Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.688	5.58 ug/L	38669	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzofuran	168	C12H8O	000132-64-9	81
2			Dibenzofuran	168	C12H8O	000132-64-9	72
3			Dibenzofuran	168	C12H8O	000132-64-9	59
4			3,5-Dimethoxybenzyl alcohol	168	C9H12O3	000705-76-0	56
5			9H-Pyrido[3,4-b]indole	168	C11H8N2	000244-63-3	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX073124\
Data File : VX042772.D
Acq On : 31 Jul 2024 14:50
Operator : JC/MD
Sample : P3348-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VHBLK001

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML072624WMA.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
Sulfur dioxide	1.239	3.6	ug/L	20753	1	6.763	290628	50.0
Azulene	13.774	19.6	ug/L	135564	3	12.024	346717	50.0
Naphthalene, 1-...	14.780	4.0	ug/L	27988	3	12.024	346717	50.0
Acenaphthene	16.328	8.9	ug/L	61589	3	12.024	346717	50.0
Dibenzofuran	16.688	5.6	ug/L	38669	3	12.024	346717	50.0