

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
 Data File : VX025600.D
 Acq On : 08 Dec 2021 00:40
 Operator : JC/MD
 Sample : M4885-06ME
 Misc : 6.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW9L3ME

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: VX025600.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	22	25	32	rBV2	4442	8476	0.83%	0.151%
2	1.368	43	46	54	rVB	62718	73717	7.18%	1.309%
3	1.648	88	92	97	rBV	37657	43536	4.24%	0.773%
4	2.282	190	196	205	rBV	112246	185762	18.08%	3.299%
5	2.788	273	279	285	rVB4	1038	2255	0.22%	0.040%
6	2.953	298	306	315	rBV	5196	13462	1.31%	0.239%
7	3.245	352	354	357	rVV	149	165	0.02%	0.003%
8	3.733	432	434	436	rVB	178	145	0.01%	0.003%
9	4.489	548	558	589	rBV	21720	104049	10.13%	1.848%
10	5.068	640	653	673	rVV2	59070	198022	19.28%	3.517%
11	5.812	773	775	780	rVB	220	244	0.02%	0.004%
12	5.970	789	801	822	rBV2	176675	519692	50.59%	9.231%
13	6.361	859	865	867	rBV4	1875	3272	0.32%	0.058%
14	6.489	883	886	888	rBV	106	140	0.01%	0.002%
15	6.550	895	896	899	rBV	171	197	0.02%	0.003%
16	6.659	912	914	917	rBV2	129	155	0.02%	0.003%
17	6.763	922	931	948	rVV	119883	308024	29.99%	5.471%
18	7.013	970	972	976	rBV2	110	154	0.01%	0.003%
19	7.129	981	991	1002	rBV	68702	156560	15.24%	2.781%
20	7.312	1013	1021	1038	rVB	99130	230262	22.42%	4.090%
21	7.421	1038	1039	1041	rBV	138	146	0.01%	0.003%
22	7.476	1046	1048	1051	rBV	294	260	0.03%	0.005%
23	8.330	1180	1188	1199	rBV	57227	106009	10.32%	1.883%
24	8.653	1234	1241	1249	rBV	265709	440793	42.91%	7.829%
25	8.958	1285	1291	1304	rVB	36903	65853	6.41%	1.170%
26	9.159	1319	1324	1330	rBV	4174	6826	0.66%	0.121%
27	9.275	1336	1343	1357	rBV	683633	1027244	100.00%	18.246%
28	9.403	1357	1364	1382	rVB	135331	227312	22.13%	4.037%
29	9.555	1388	1389	1394	rVB2	276	305	0.03%	0.005%
30	9.622	1396	1400	1405	rVV2	480	653	0.06%	0.012%
31	9.714	1412	1415	1419	rVV	627	932	0.09%	0.017%
32	9.817	1428	1432	1435	rBV2	106	170	0.02%	0.003%
33	10.061	1465	1472	1480	rBV	246145	365493	35.58%	6.492%
34	10.201	1491	1495	1501	rVB2	701	1063	0.10%	0.019%
35	10.305	1507	1512	1519	rVV	4538	6669	0.65%	0.118%
36	10.354	1519	1520	1525	rVB2	238	152	0.01%	0.003%

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Integrator: RTE

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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	10.646	1564	1568	1573	rVB2	2280	2940	0.29%	0.052%
38	10.762	1584	1587	1589	rBV3	217	289	0.03%	0.005%
39	10.896	1607	1609	1611	rVB2	230	245	0.02%	0.004%
40	11.122	1640	1646	1651	rVB	3416	4414	0.43%	0.078%
41	11.195	1653	1658	1665	rBV	177991	238897	23.26%	4.243%
42	11.384	1686	1689	1692	rBV2	426	492	0.05%	0.009%
43	11.476	1697	1704	1707	rBV2	1422	2859	0.28%	0.051%
44	11.549	1714	1716	1720	rVB2	349	401	0.04%	0.007%
45	11.622	1725	1728	1731	rBV2	286	372	0.04%	0.007%
46	11.719	1740	1744	1745	rBV3	610	788	0.08%	0.014%
47	11.750	1745	1749	1754	rVB2	3769	5470	0.53%	0.097%
48	11.841	1762	1764	1767	rVB2	566	602	0.06%	0.011%
49	11.933	1775	1779	1784	rBV	1696	2240	0.22%	0.040%
50	12.024	1789	1794	1800	rBV	309363	380050	37.00%	6.750%
51	12.152	1812	1815	1819	rVB2	2691	3125	0.30%	0.056%
52	12.225	1826	1827	1830	rBV2	150	210	0.02%	0.004%
53	12.274	1830	1835	1836	rVV3	366	558	0.05%	0.010%
54	12.323	1836	1843	1849	rVV	326725	405715	39.50%	7.206%
55	12.427	1856	1860	1864	rVB3	1776	2385	0.23%	0.042%
56	12.481	1864	1869	1873	rBV5	551	1042	0.10%	0.019%
57	12.616	1889	1891	1895	rVB2	337	379	0.04%	0.007%
58	12.664	1896	1899	1900	rBV3	476	392	0.04%	0.007%
59	12.853	1928	1930	1932	rBV	294	178	0.02%	0.003%
60	12.884	1932	1935	1937	rVV2	310	310	0.03%	0.006%
61	12.927	1939	1942	1945	rVB3	363	452	0.04%	0.008%
62	12.969	1945	1949	1952	rBV2	1087	1253	0.12%	0.022%
63	13.048	1958	1962	1967	rBV4	570	813	0.08%	0.014%
64	13.268	1994	1998	1999	rBV3	1245	1216	0.12%	0.022%
65	13.384	2015	2017	2019	rVB2	340	296	0.03%	0.005%
66	13.500	2034	2036	2039	rBV	134	142	0.01%	0.003%
67	13.579	2045	2049	2055	rBV2	438	612	0.06%	0.011%
68	13.676	2062	2065	2066	rBV2	189	162	0.02%	0.003%
69	13.780	2075	2082	2089	rBV	29524	39350	3.83%	0.699%
70	13.841	2089	2092	2096	rBV4	476	661	0.06%	0.012%
71	13.926	2103	2106	2111	rVB4	123	210	0.02%	0.004%
72	13.975	2111	2114	2117	rVB	207	245	0.02%	0.004%
73	14.018	2117	2121	2122	rBV2	241	273	0.03%	0.005%
74	14.036	2122	2124	2128	rVB3	1129	1350	0.13%	0.024%
75	14.085	2128	2132	2135	rVB3	329	453	0.04%	0.008%
76	14.134	2139	2140	2142	rVV2	256	189	0.02%	0.003%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Peak Location: TOP

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

77	14.152	2142	2143	2146	rVV	327	212	0.02%	0.004%
78	14.213	2150	2153	2159	rBV2	407	583	0.06%	0.010%
79	14.323	2169	2171	2174	rVB	520	370	0.04%	0.007%
80	14.371	2176	2179	2183	rVB4	627	580	0.06%	0.010%
81	14.445	2189	2191	2194	rVB2	357	332	0.03%	0.006%
82	14.481	2194	2197	2199	rBV2	359	454	0.04%	0.008%
83	14.499	2199	2200	2206	rVB3	454	643	0.06%	0.011%
84	14.566	2207	2211	2215	rBV3	1270	1971	0.19%	0.035%
85	14.640	2218	2223	2234	rVB	43111	54345	5.29%	0.965%
86	14.780	2234	2246	2254	rBV	51938	68729	6.69%	1.221%
87	15.024	2284	2286	2288	rBV2	260	253	0.02%	0.004%
88	15.079	2293	2295	2298	rBV3	380	419	0.04%	0.007%
89	15.207	2305	2316	2321	rBV2	6782	11170	1.09%	0.198%
90	15.377	2333	2344	2347	rBV4	4364	8454	0.82%	0.150%
91	15.414	2347	2350	2354	rVV5	3446	4694	0.46%	0.083%
92	15.481	2355	2361	2371	rVB	40984	67499	6.57%	1.199%
93	15.615	2378	2383	2386	rBV	65451	95389	9.29%	1.694%
94	15.737	2401	2403	2409	rVB3	1113	1369	0.13%	0.024%
95	15.841	2409	2420	2429	rBV	19848	53712	5.23%	0.954%
96	15.987	2439	2444	2453	rVB	9104	15459	1.50%	0.275%
97	16.097	2456	2462	2468	rVB	11785	19823	1.93%	0.352%
98	16.200	2475	2479	2483	rVB4	1545	2412	0.23%	0.043%
99	16.597	2540	2544	2550	rVB3	5993	9176	0.89%	0.163%
100	16.664	2550	2555	2557	rBV3	6869	11857	1.15%	0.211%

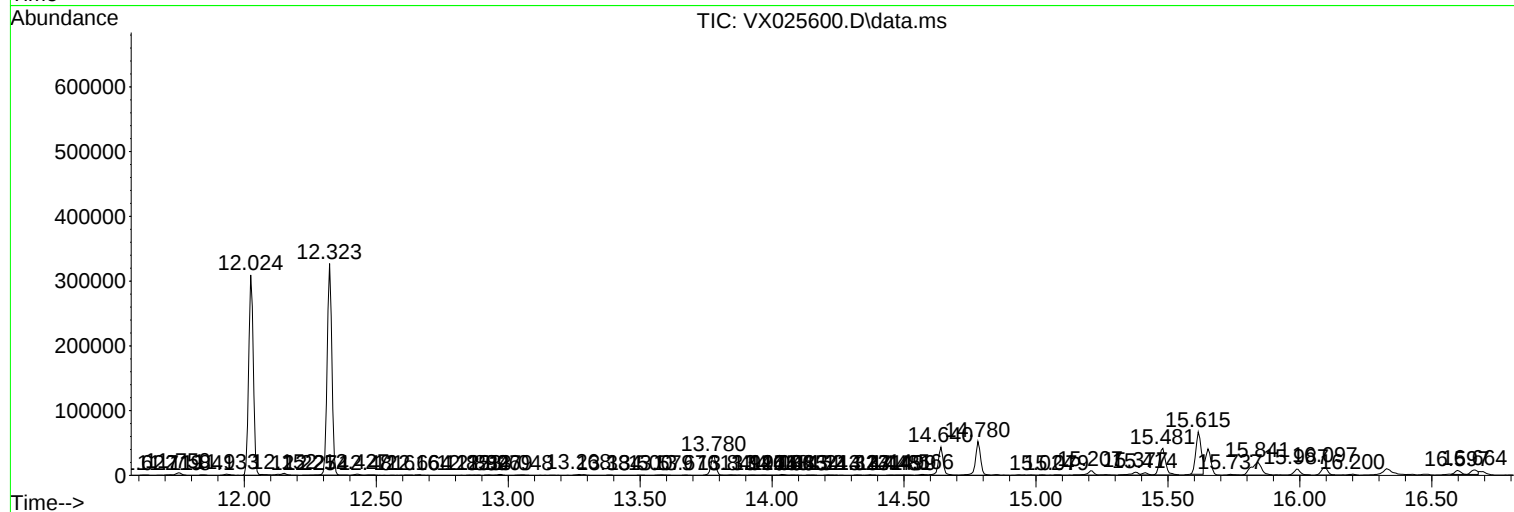
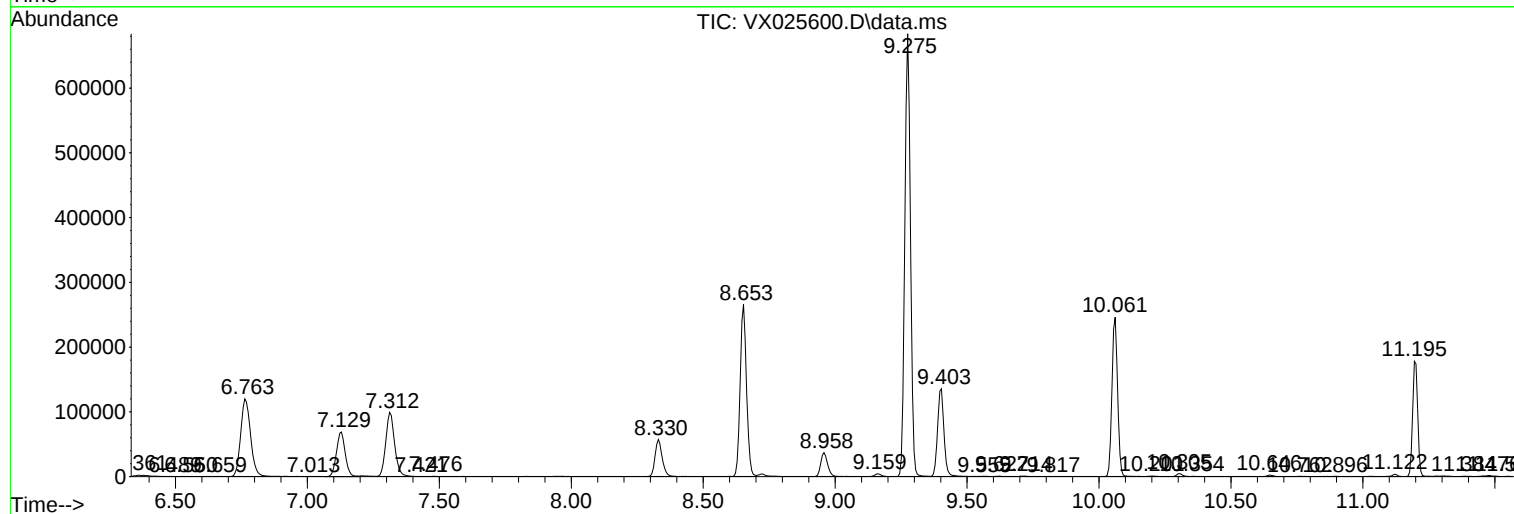
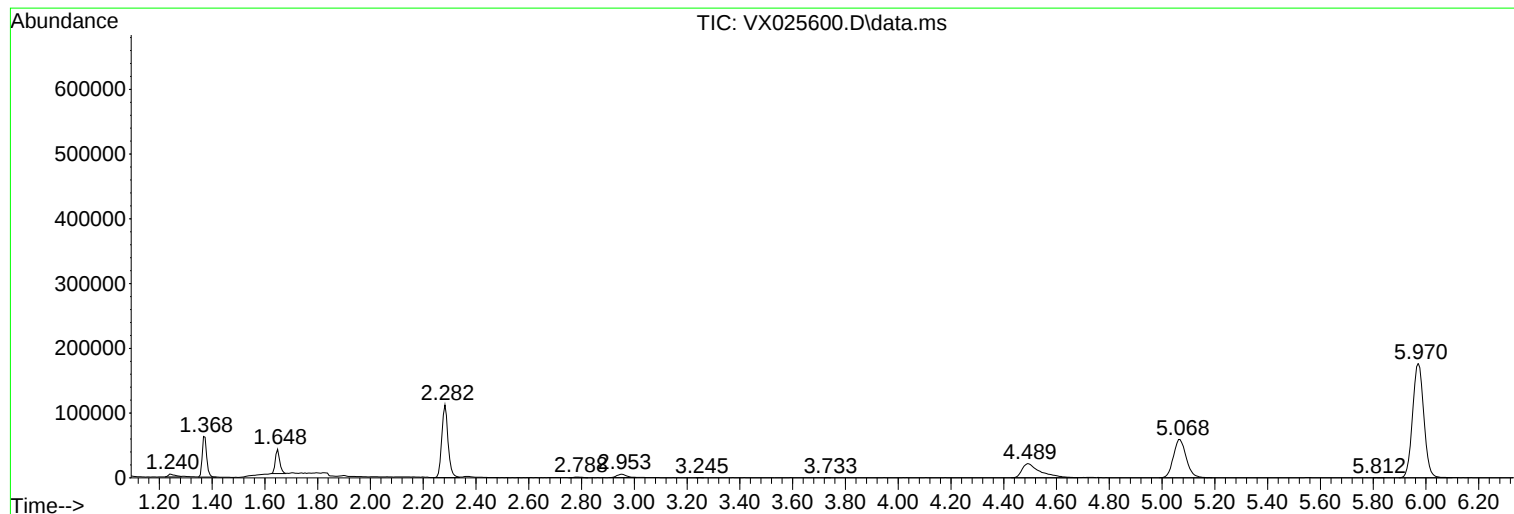
Sum of corrected areas: 5630104

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Instrument :
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ClientSampleId :
EW9L3ME

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



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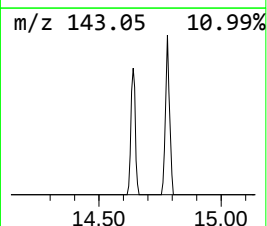
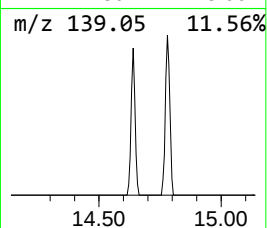
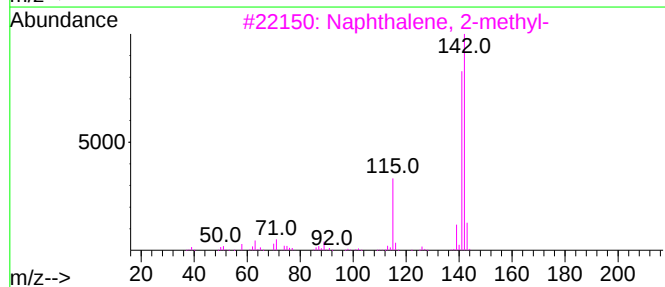
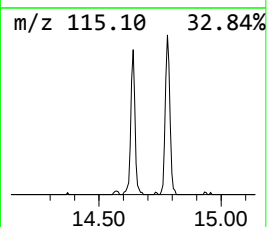
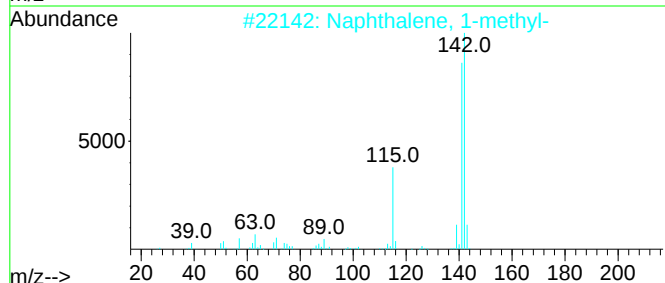
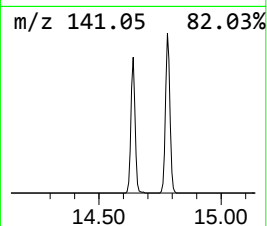
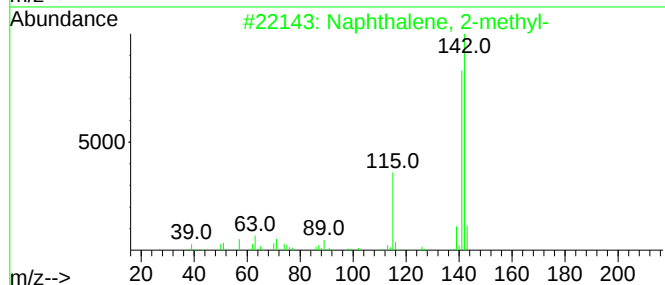
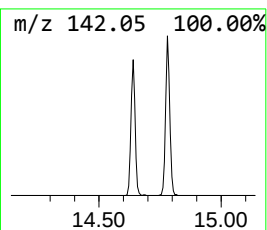
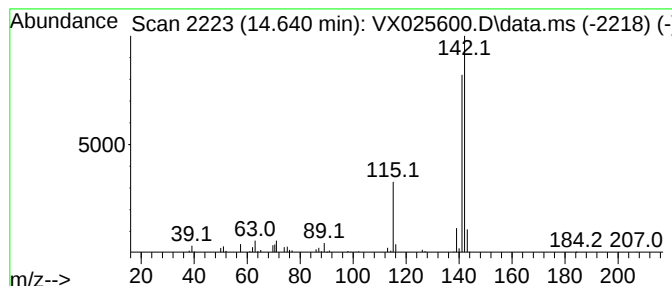
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML112221WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Naphthalene, 1-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	7.15 ug/L	54345	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	94
5			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91



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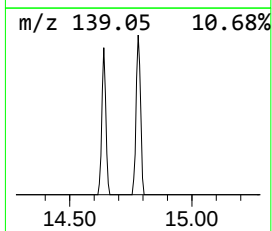
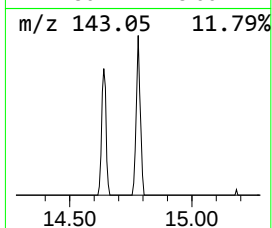
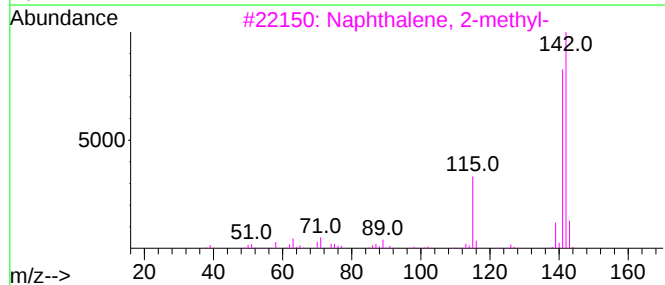
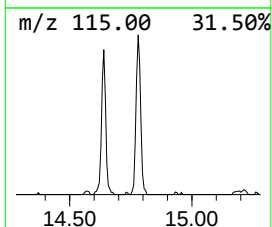
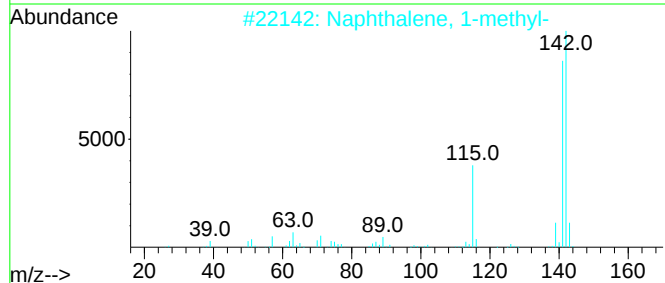
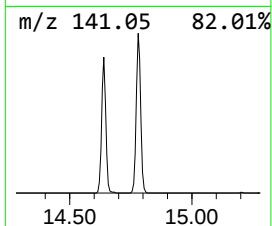
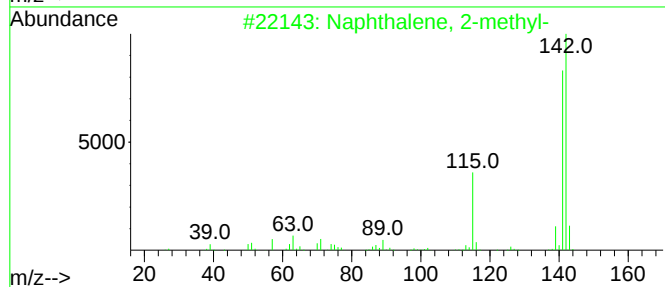
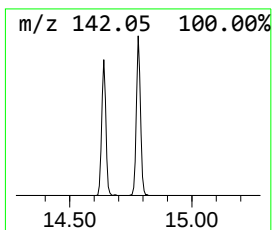
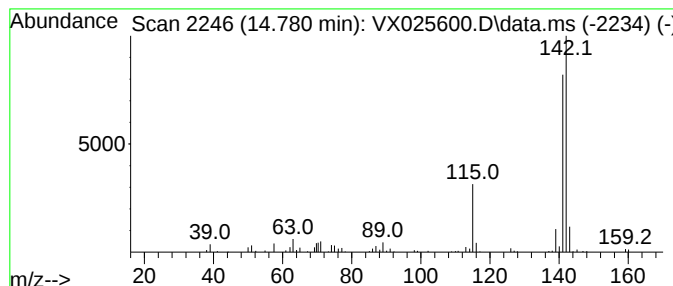
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML112221WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	9.04 ug/L	68729	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	97
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	97
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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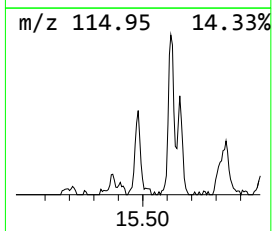
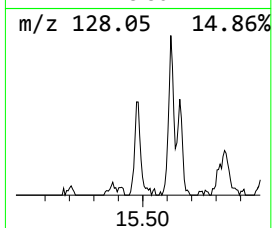
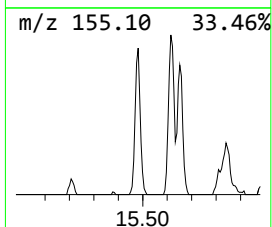
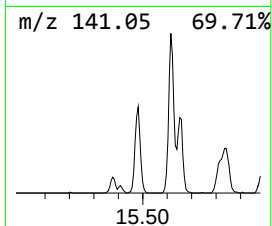
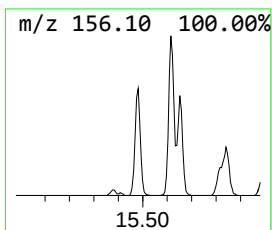
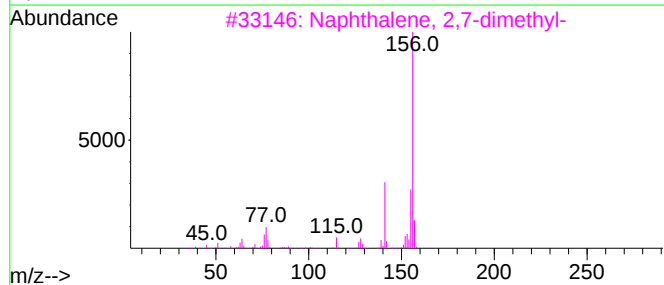
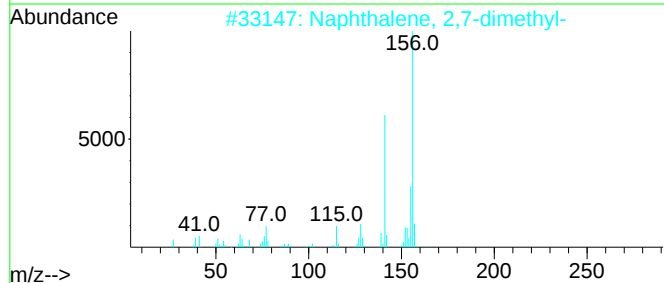
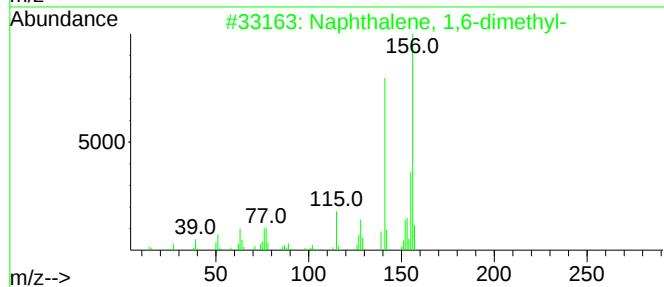
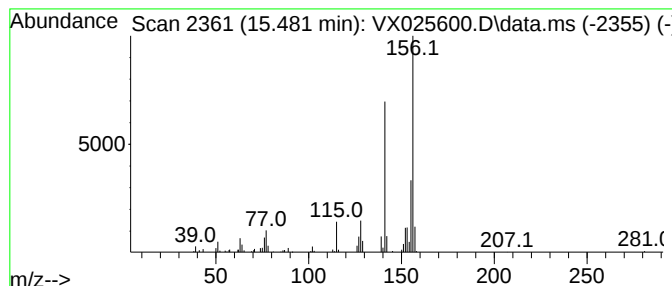
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Quant Title : VOC Analysis

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

Peak Number 5 Naphthalene, 1,6-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.481	8.88 ug/L	67499	1,4-Dichlorobenzene-d4	12.024

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025600.D
Acq On : 08 Dec 2021 00:40
Operator : JC/MD
Sample : M4885-06ME
Misc : 6.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9L3ME

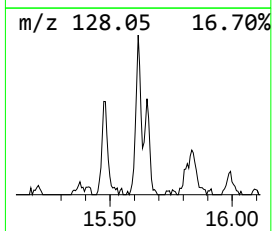
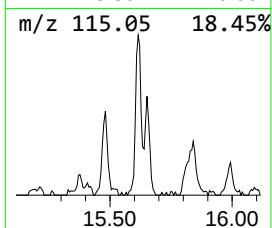
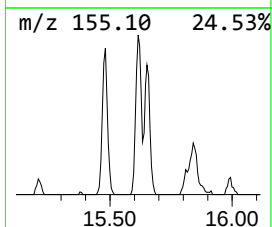
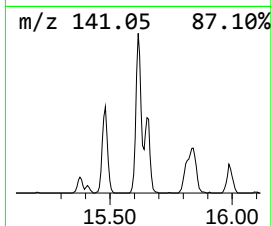
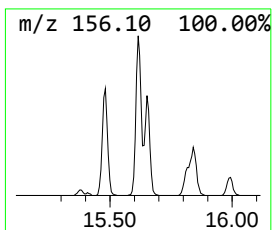
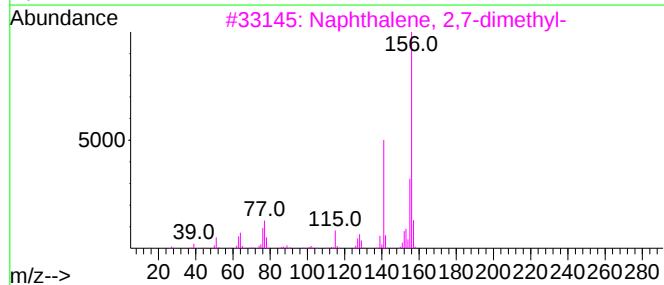
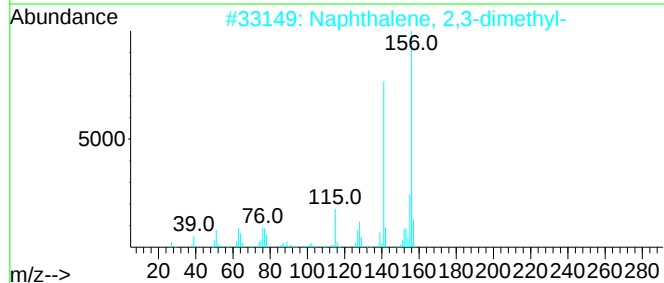
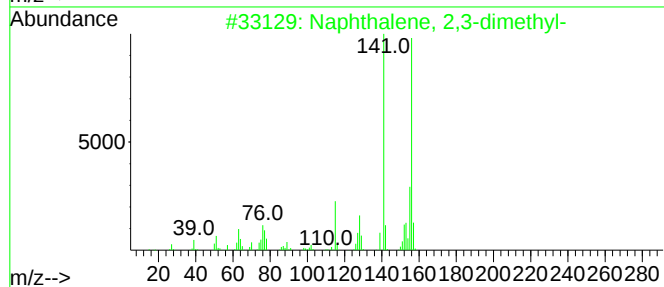
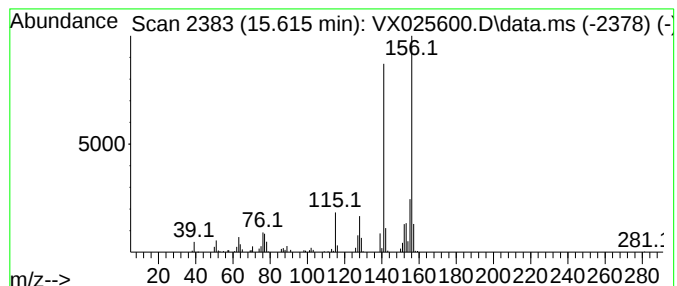
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Quant Title : VOC Analysis

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

Peak Number 6 Naphthalene, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.615	12.55 ug/L	95389	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	98
2			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
3			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	97
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
5			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025600.D
Acq On : 08 Dec 2021 00:40
Operator : JC/MD
Sample : M4885-06ME
Misc : 6.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9L3ME

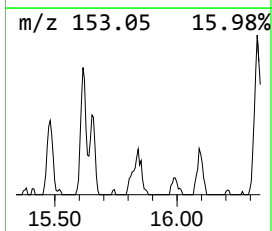
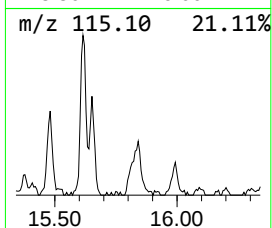
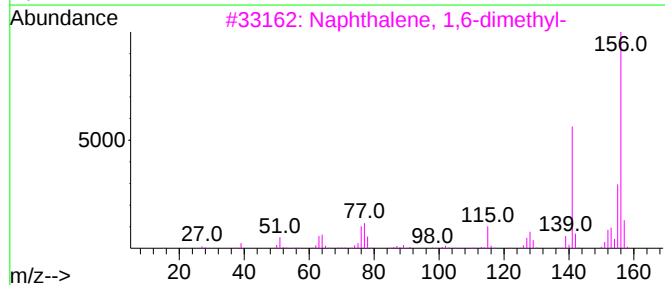
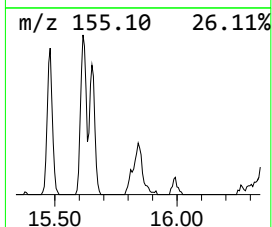
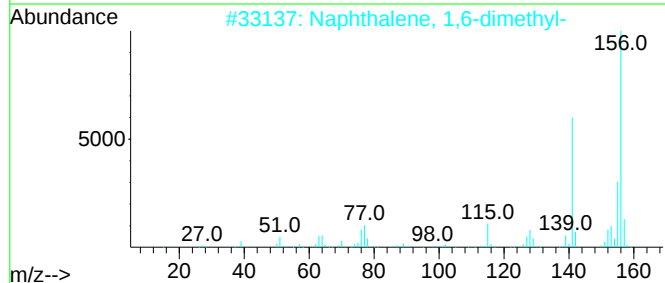
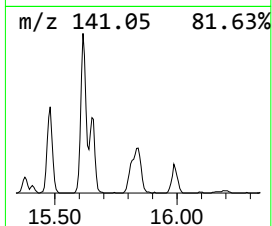
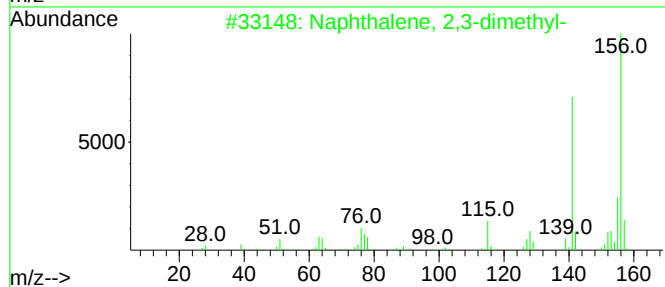
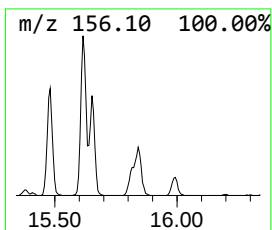
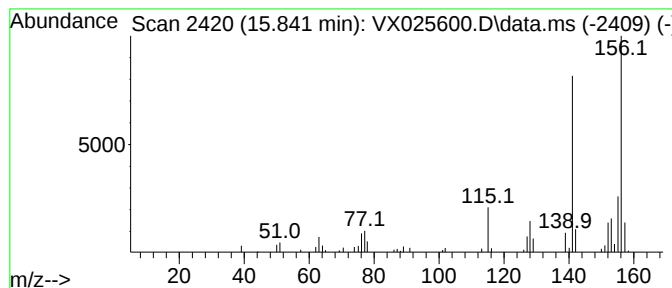
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Quant Title : VOC Analysis

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

Peak Number 7 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.841	7.07 ug/L	53712	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
2			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
4			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
5			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025600.D
Acq On : 08 Dec 2021 00:40
Operator : JC/MD
Sample : M4885-06ME
Misc : 6.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9L3ME

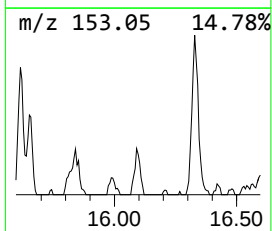
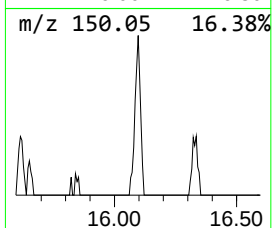
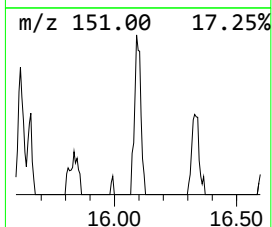
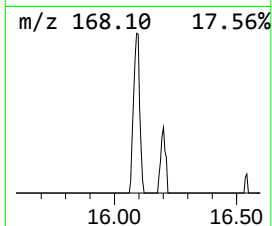
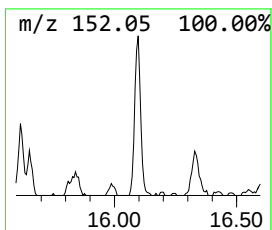
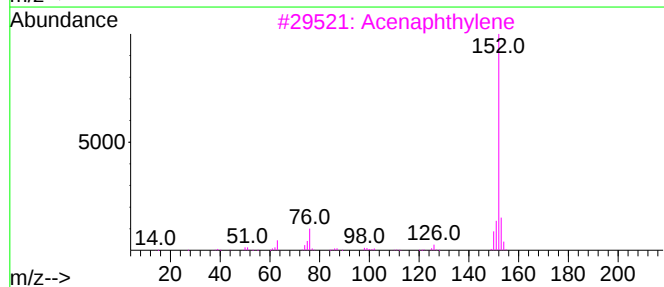
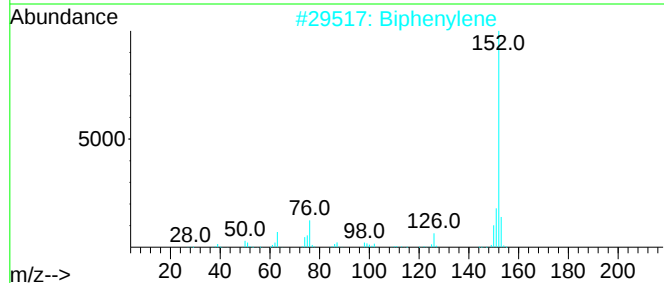
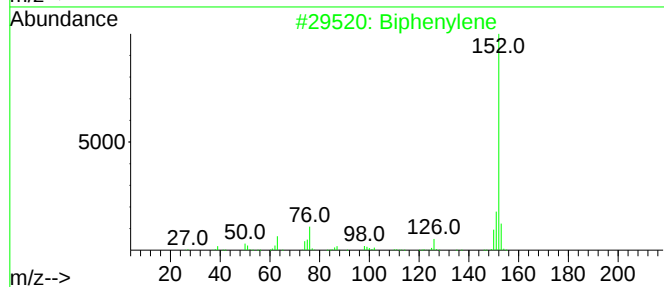
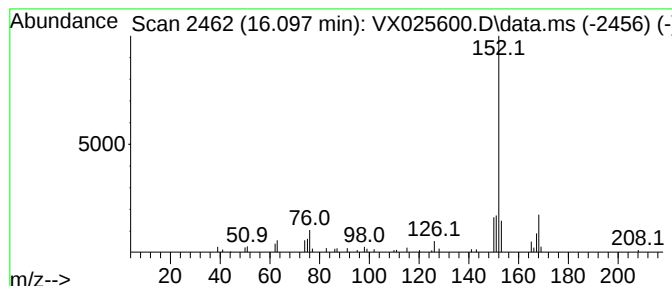
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Quant Title : VOC Analysis

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

Peak Number 8 Biphenylene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.097	2.61 ug/L	19823	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Biphenylene	152	C12H8	000259-79-0	95
2			Biphenylene	152	C12H8	000259-79-0	93
3			Acenaphthylene	152	C12H8	000208-96-8	83
4			Acenaphthylene	152	C12H8	000208-96-8	76
5			(6Balpha,7beta,11alpha,11aalpha)...	334	C25H18O	1000241-69-8	72



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
Data File : VX025600.D
Acq On : 08 Dec 2021 00:40
Operator : JC/MD
Sample : M4885-06ME
Misc : 6.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 37 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9L3ME

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Naphthalene, 1-...	14.640	7.2	ug/L	54345	3	12.024	380050	50.0
unknown-01	14.780	9.0	ug/L	68729	3	12.024	380050	50.0
Naphthalene, 1,...	15.481	8.9	ug/L	67499	3	12.024	380050	50.0
Naphthalene, 2,...	15.615	12.6	ug/L	95389	3	12.024	380050	50.0
unknown-02	15.841	7.1	ug/L	53712	3	12.024	380050	50.0
Biphenylene	16.097	2.6	ug/L	19823	3	12.024	380050	50.0