

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101921\
 Data File : VX024845.D
 Acq On : 19 Oct 2021 13:56
 Operator : JC/MD
 Sample : M4181-14ME
 Misc : 5.60g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AZ2ME

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\SFAMXML100721WMA.M

Title : VOC Analysis

Signal : TIC: VX024845.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	43	46	53	rVB	113718	134535	10.78%	1.239%
2	1.648	89	92	100	rBV	73010	99136	7.94%	0.913%
3	2.276	188	195	204	rBV	226038	362987	29.07%	3.344%
4	2.373	206	211	220	rVV2	5068	12605	1.01%	0.116%
5	2.751	260	273	276	rBV4	4544	12258	0.98%	0.113%
6	2.995	311	313	319	rVB4	650	1039	0.08%	0.010%
7	3.075	319	326	334	rBV2	6107	14748	1.18%	0.136%
8	3.410	377	381	382	rBV2	1742	1716	0.14%	0.016%
9	3.727	430	433	437	rBV3	342	728	0.06%	0.007%
10	4.190	504	509	510	rBV2	1039	1499	0.12%	0.014%
11	4.288	517	525	537	rVB3	9528	25575	2.05%	0.236%
12	4.495	548	559	578	rBV2	85372	363182	29.09%	3.346%
13	5.062	638	652	666	rBV	165244	507491	40.65%	4.675%
14	5.379	701	704	708	rBV3	993	1895	0.15%	0.017%
15	5.464	708	718	731	rVV6	13011	51839	4.15%	0.478%
16	5.617	735	743	750	rVB6	3775	10481	0.84%	0.097%
17	5.830	769	778	786	rBV6	5084	14765	1.18%	0.136%
18	5.970	789	801	816	rBV2	444535	1248560	100.00%	11.502%
19	6.153	824	831	832	rBV3	4415	8827	0.71%	0.081%
20	6.354	854	864	878	rVB6	12738	39617	3.17%	0.365%
21	6.611	899	906	916	rVB6	3425	7539	0.60%	0.069%
22	6.763	921	931	946	rBV	286119	695611	55.71%	6.408%
23	6.891	949	952	954	rVB2	769	885	0.07%	0.008%
24	7.110	980	988	999	rBV4	7971	20463	1.64%	0.189%
25	7.220	1000	1006	1012	rBV4	2591	5827	0.47%	0.054%
26	7.312	1012	1021	1027	rBV	262439	580432	46.49%	5.347%
27	7.488	1043	1050	1051	rBV5	1963	3518	0.28%	0.032%
28	7.653	1072	1077	1084	rVB6	3708	7852	0.63%	0.072%
29	7.714	1084	1087	1090	rBV2	465	784	0.06%	0.007%
30	7.775	1090	1097	1111	rVB4	8274	18718	1.50%	0.172%
31	7.958	1119	1127	1136	rVB5	10511	22989	1.84%	0.212%
32	8.189	1160	1165	1167	rBV5	1657	2599	0.21%	0.024%
33	8.275	1174	1179	1182	rBV3	6563	10430	0.84%	0.096%
34	8.330	1182	1188	1201	rVB	175675	297322	23.81%	2.739%
35	8.433	1202	1205	1209	rVB4	2843	4146	0.33%	0.038%
36	8.604	1226	1233	1234	rBV4	13932	22622	1.81%	0.208%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101921\
 Data File : VX024845.D
 Acq On : 19 Oct 2021 13:56
 Operator : JC/MD
 Sample : M4181-14ME
 Misc : 5.60g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AZ2ME

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\SFAMXLM100721WMA.M
 Title : VOC Analysis

37	8.653	1235	1241	1247	rVV	593191	969911	77.68%	8.935%
38	8.720	1248	1252	1256	rVV	28524	40231	3.22%	0.371%
39	8.909	1279	1283	1285	rBV2	5846	7880	0.63%	0.073%
40	8.952	1285	1290	1305	rVB	135403	230397	18.45%	2.122%
41	9.104	1308	1315	1320	rBV3	5671	10362	0.83%	0.095%
42	9.208	1328	1332	1334	rBV4	1934	2804	0.22%	0.026%
43	9.269	1337	1342	1352	rVB5	2005	3863	0.31%	0.036%
44	9.397	1357	1363	1377	rBV	363922	753443	60.34%	6.941%
45	9.512	1378	1382	1386	rBV6	4522	6150	0.49%	0.057%
46	9.567	1386	1391	1395	rVB	17351	26232	2.10%	0.242%
47	9.622	1395	1400	1403	rBV3	10117	16630	1.33%	0.153%
48	9.762	1418	1423	1428	rVB3	3716	5769	0.46%	0.053%
49	9.817	1428	1432	1440	rBV5	8755	18793	1.51%	0.173%
50	9.909	1443	1447	1450	rVV5	4495	5840	0.47%	0.054%
51	10.006	1458	1463	1466	rBV5	4526	7350	0.59%	0.068%
52	10.055	1466	1471	1479	rVV	578015	800698	64.13%	7.376%
53	10.195	1490	1494	1499	rVB2	11991	15738	1.26%	0.145%
54	10.305	1508	1512	1517	rVB	35965	50750	4.06%	0.468%
55	10.360	1517	1521	1530	rVB3	16469	26083	2.09%	0.240%
56	10.457	1533	1537	1543	rVB4	2244	3480	0.28%	0.032%
57	10.592	1551	1559	1564	rBV7	6712	13727	1.10%	0.126%
58	10.646	1564	1568	1574	rVB	38354	52389	4.20%	0.483%
59	10.756	1581	1586	1587	rBV	7689	9605	0.77%	0.088%
60	10.860	1598	1603	1606	rBV2	11557	17110	1.37%	0.158%
61	10.896	1606	1609	1615	rVB2	10767	16280	1.30%	0.150%
62	10.963	1616	1620	1624	rBV	12206	16330	1.31%	0.150%
63	11.122	1642	1646	1651	rVB4	7347	12288	0.98%	0.113%
64	11.195	1653	1658	1670	rBV	480454	676586	54.19%	6.233%
65	11.305	1673	1676	1679	rBV	10154	12495	1.00%	0.115%
66	11.384	1685	1689	1695	rVB5	13279	22520	1.80%	0.207%
67	11.482	1702	1705	1710	rVB2	19065	23822	1.91%	0.219%
68	11.616	1723	1727	1735	rBV2	11249	16617	1.33%	0.153%
69	11.677	1735	1737	1738	rBV	1318	767	0.06%	0.007%
70	11.713	1740	1743	1746	rVV3	11401	14664	1.17%	0.135%
71	11.756	1746	1750	1760	rVB	36419	54698	4.38%	0.504%
72	11.866	1761	1768	1769	rBV6	5098	9401	0.75%	0.087%
73	11.896	1770	1773	1776	rVB3	7748	10421	0.83%	0.096%
74	12.024	1789	1794	1800	rBV	657408	822454	65.87%	7.577%
75	12.091	1802	1805	1813	rVB2	14276	23290	1.87%	0.215%
76	12.250	1828	1831	1832	rBV3	2755	3289	0.26%	0.030%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101921\
 Data File : VX024845.D
 Acq On : 19 Oct 2021 13:56
 Operator : JC/MD
 Sample : M4181-14ME
 Misc : 5.60g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AZ2ME

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\SFAMXML100721WMA.M
 Title : VOC Analysis

77	12.323	1838	1843	1851	rVB	759680	970502	77.73%	8.941%
78	12.427	1856	1860	1864	rVV	22517	27080	2.17%	0.249%
79	12.536	1875	1878	1880	rBV3	5870	7401	0.59%	0.068%
80	12.890	1933	1936	1939	rBV5	5229	6773	0.54%	0.062%
81	12.975	1946	1950	1956	rVB6	6871	11098	0.89%	0.102%
82	13.036	1956	1960	1964	rBV6	3461	6518	0.52%	0.060%
83	13.268	1995	1998	2007	rVB2	19061	31866	2.55%	0.294%
84	13.384	2015	2017	2021	rVB3	6627	8460	0.68%	0.078%
85	13.518	2033	2039	2041	rBV6	2679	4889	0.39%	0.045%
86	13.579	2047	2049	2054	rBV4	4520	6315	0.51%	0.058%
87	13.780	2078	2082	2088	rVB	52229	70772	5.67%	0.652%
88	13.847	2089	2093	2097	rVB3	10921	13999	1.12%	0.129%
89	13.877	2097	2098	2100	rBV2	1867	1366	0.11%	0.013%
90	14.042	2121	2125	2128	rBV	13179	15768	1.26%	0.145%
91	14.109	2132	2136	2140	rVB7	5853	8384	0.67%	0.077%
92	14.640	2219	2223	2227	rVB	54693	59923	4.80%	0.552%
93	14.780	2240	2246	2253	rVB	51291	76710	6.14%	0.707%
94	15.127	2299	2303	2307	rBV5	11397	16173	1.30%	0.149%
95	15.377	2342	2344	2349	rVB5	6217	5696	0.46%	0.052%
96	15.481	2355	2361	2370	rBV3	11277	24565	1.97%	0.226%
97	15.615	2379	2383	2387	rBV	17246	26674	2.14%	0.246%
98	16.091	2456	2461	2464	rBV6	2896	4793	0.38%	0.044%
99	16.426	2514	2516	2517	rBV2	1512	1098	0.09%	0.010%
100	16.657	2551	2554	2556	rBV4	1470	1849	0.15%	0.017%

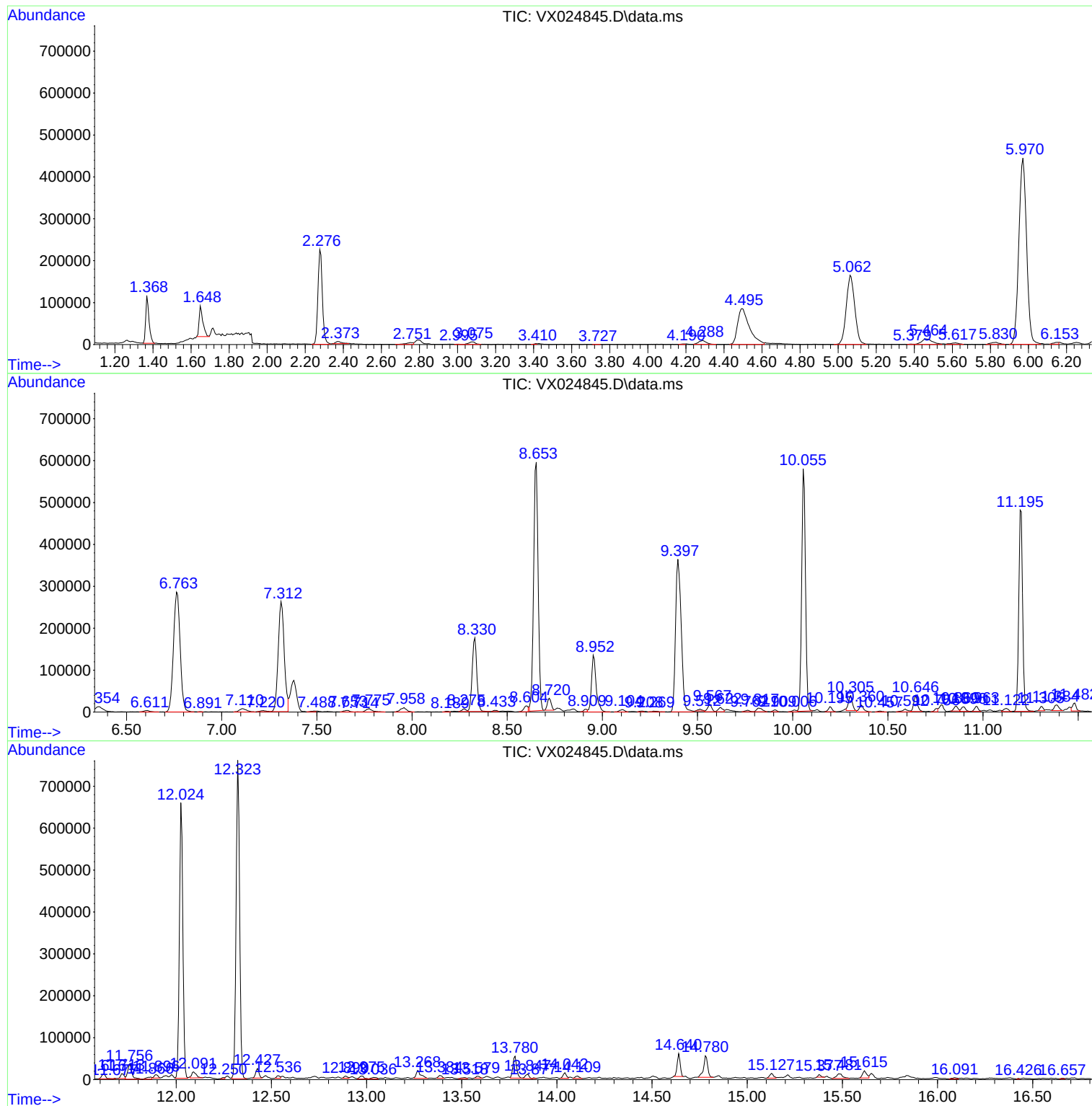
Sum of corrected areas: 10855049

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101921\
Data File : VX024845.D
Acq On : 19 Oct 2021 13:56
Operator : JC/MD
Sample : M4181-14ME
Misc : 5.60g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AZ2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM100721WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101921\
Data File : VX024845.D
Acq On : 19 Oct 2021 13:56
Operator : JC/MD
Sample : M4181-14ME
Misc : 5.60g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AZ2ME

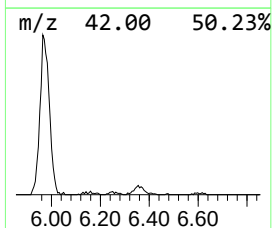
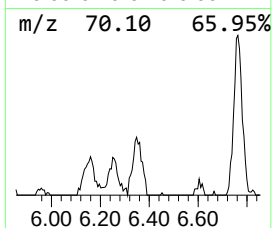
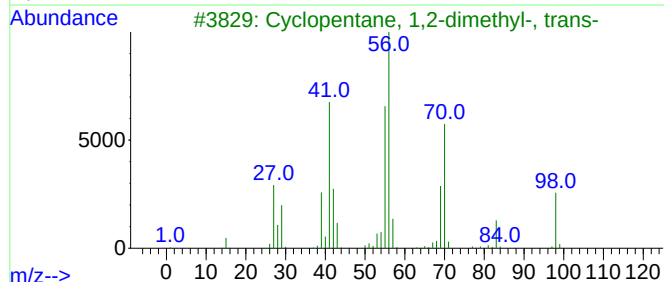
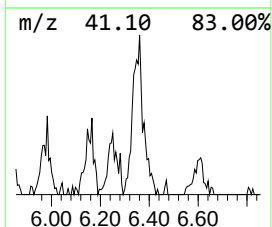
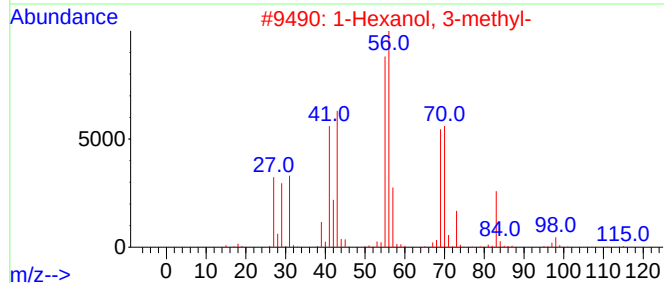
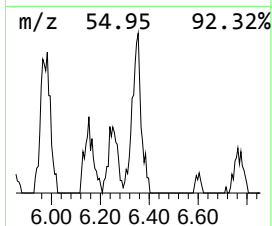
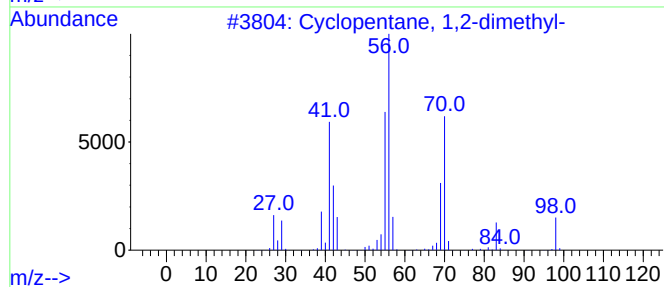
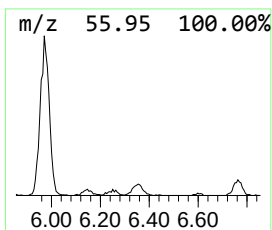
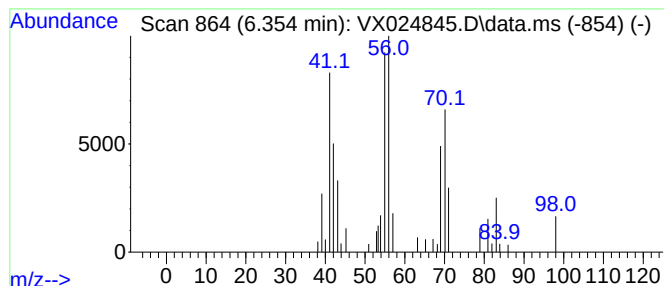
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM100721WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Cyclic6.354 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.354	2.85 ug/L	39617	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	58
2		1-Hexanol, 3-methyl-	116	C7H16O	013231-81-7	53
3		Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	53
4		1-Heptene	98	C7H14	000592-76-7	53
5		2,3-Dimethyl-aziridine	71	C4H9N	002549-68-0	52



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101921\
Data File : VX024845.D
Acq On : 19 Oct 2021 13:56
Operator : JC/MD
Sample : M4181-14ME
Misc : 5.60g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AZ2ME

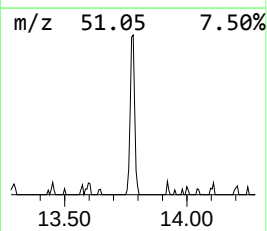
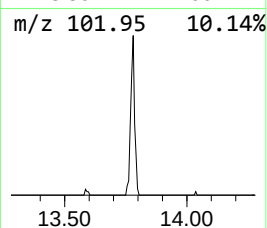
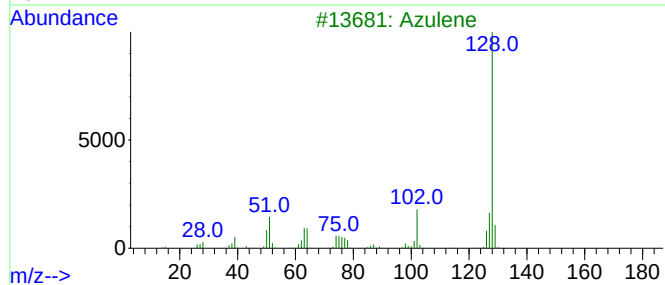
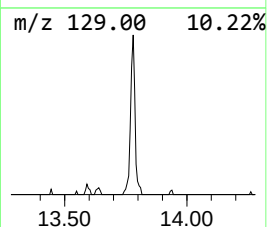
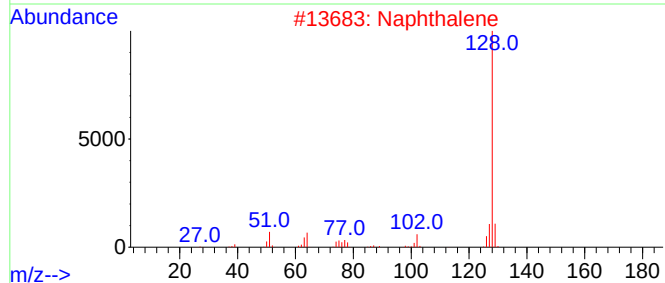
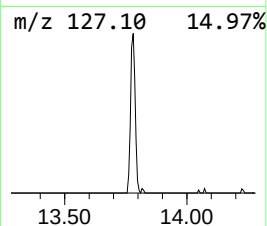
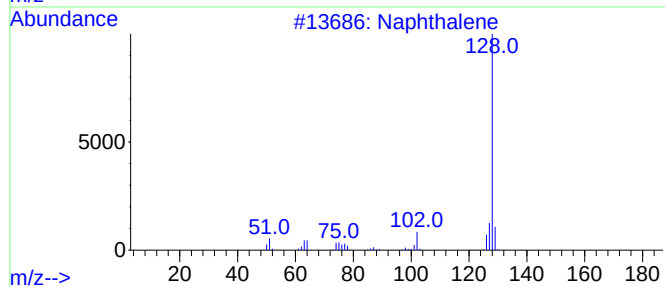
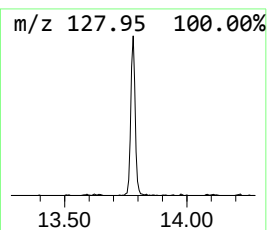
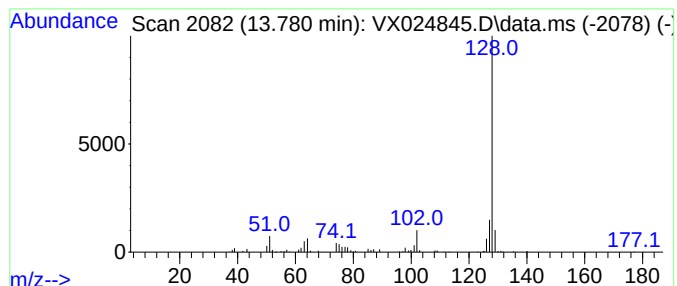
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM100721WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	4.30 ug/L	70772	1,4-Dichlorobenzene-d4	12.024

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	94
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101921\
Data File : VX024845.D
Acq On : 19 Oct 2021 13:56
Operator : JC/MD
Sample : M4181-14ME
Misc : 5.60g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AZ2ME

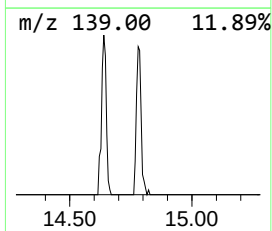
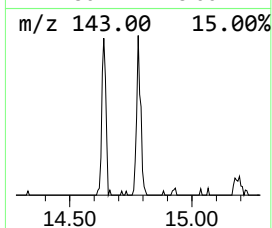
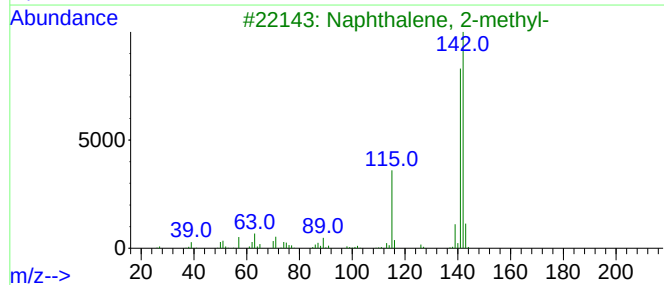
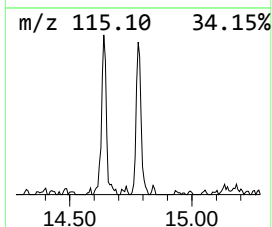
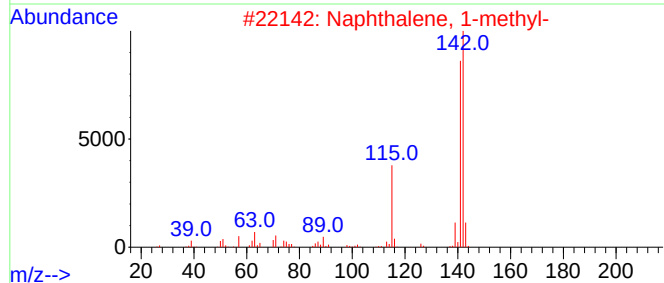
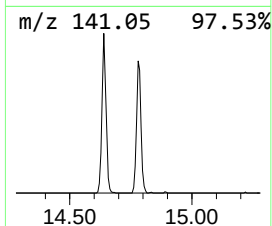
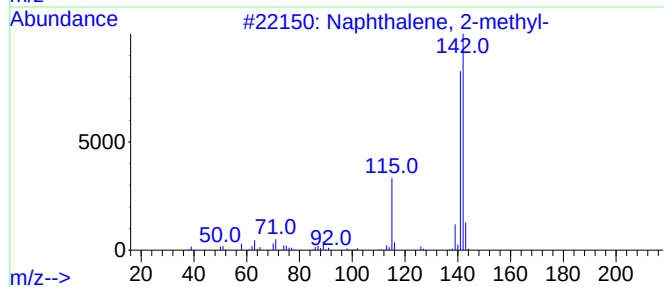
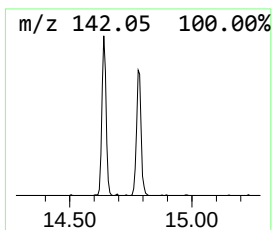
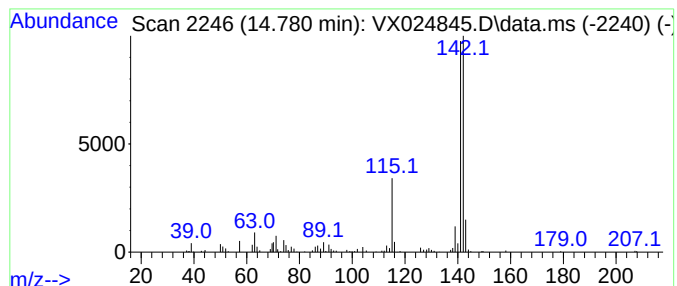
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM100721WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 1H-Indene, 1-ethylidene- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.780	4.66 ug/L	76710	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	96
3			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
4			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	95
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	95



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX101921\
Data File : VX024845.D
Acq On : 19 Oct 2021 13:56
Operator : JC/MD
Sample : M4181-14ME
Misc : 5.60g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AZ2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML100721WMA.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
(DEL) Alkane: C...	6.354	2.9	ug/L	39617	1	6.763	695611	50.0
Azulene	13.780	4.3	ug/L	70772	3	12.024	822454	50.0
1H-Indene, 1-et...	14.780	4.7	ug/L	76710	3	12.024	822454	50.0