

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
 Data File : VX025630.D
 Acq On : 08 Dec 2021 19:30
 Operator : JC/MD
 Sample : M4883-17ME
 Misc : 2.78g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW9H3ME

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\SFAMXML112221WMA.M
 Title : VOC Analysis

Signal : TIC: VX025630.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	22	26	27	rBV	4525	5885	1.00%	0.110%
2	1.374	43	47	53	rVB	68468	79003	13.38%	1.474%
3	1.648	89	92	98	rVB	41151	49806	8.44%	0.930%
4	1.709	99	102	108	rVV	11443	13059	2.21%	0.244%
5	2.282	190	196	206	rBV	121683	202313	34.27%	3.776%
6	2.758	263	274	275	rBV4	2391	6045	1.02%	0.113%
7	2.953	298	306	316	rBV2	3090	8126	1.38%	0.152%
8	3.081	321	327	334	rVB4	3846	8179	1.39%	0.153%
9	3.428	378	384	388	rVV4	1120	2164	0.37%	0.040%
10	4.288	516	525	533	rBV4	7886	22592	3.83%	0.422%
11	4.495	548	559	585	rBV2	24968	120124	20.35%	2.242%
12	5.068	641	653	671	rVB	72955	232131	39.32%	4.332%
13	5.464	707	718	732	rBV6	7053	24130	4.09%	0.450%
14	5.605	735	741	744	rBV4	1749	3498	0.59%	0.065%
15	5.812	769	775	784	rVB5	2304	6699	1.13%	0.125%
16	5.970	790	801	820	rVB2	201584	590355	100.00%	11.018%
17	6.147	822	830	840	rVV6	4324	12737	2.16%	0.238%
18	6.251	840	847	854	rVB3	3786	9764	1.65%	0.182%
19	6.348	856	863	875	rVB6	8240	24648	4.18%	0.460%
20	6.611	898	906	911	rBV6	1229	2987	0.51%	0.056%
21	6.763	921	931	948	rBV	140731	365670	61.94%	6.825%
22	7.117	983	989	998	rVB6	2453	6405	1.08%	0.120%
23	7.220	1001	1006	1013	rBV5	880	2028	0.34%	0.038%
24	7.312	1013	1021	1027	rBV	110156	258474	43.78%	4.824%
25	7.549	1057	1060	1065	rBV2	656	970	0.16%	0.018%
26	7.653	1070	1077	1082	rVV4	3324	6109	1.03%	0.114%
27	7.775	1090	1097	1103	rVV3	4648	8844	1.50%	0.165%
28	7.952	1121	1126	1133	rVV5	4881	9994	1.69%	0.187%
29	8.190	1160	1165	1168	rBV3	587	1071	0.18%	0.020%
30	8.275	1175	1179	1182	rBV	2458	3721	0.63%	0.069%
31	8.330	1182	1188	1200	rVB	70051	125300	21.22%	2.338%
32	8.427	1202	1204	1210	rBV4	1228	2246	0.38%	0.042%
33	8.598	1227	1232	1234	rBV2	6093	9674	1.64%	0.181%
34	8.653	1234	1241	1248	rVV	300547	506753	85.84%	9.458%
35	8.720	1248	1252	1257	rVB	13952	20951	3.55%	0.391%
36	8.769	1257	1260	1264	rVB3	3545	5021	0.85%	0.094%

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Instrument :
 MSVOA_X
 ClientSampleId :
 EW9H3ME

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

37	8.824	1265	1269	1270	rBV3	1754	2358	0.40%	0.044%
38	8.915	1279	1284	1286	rBV2	2562	3601	0.61%	0.067%
39	8.958	1286	1291	1301	rVB	46312	89972	15.24%	1.679%
40	9.098	1311	1314	1319	rBV2	2222	3513	0.60%	0.066%
41	9.202	1327	1331	1338	rBV3	1413	2236	0.38%	0.042%
42	9.275	1338	1343	1350	rBV	11010	15803	2.68%	0.295%
43	9.403	1355	1364	1374	rBV	155392	265071	44.90%	4.947%
44	9.519	1378	1383	1386	rBV5	2320	3890	0.66%	0.073%
45	9.561	1386	1390	1395	rVB	8287	12040	2.04%	0.225%
46	9.622	1395	1400	1403	rBV3	4833	8218	1.39%	0.153%
47	9.762	1419	1423	1427	rBV3	1461	2357	0.40%	0.044%
48	9.823	1428	1433	1438	rVB5	3279	6188	1.05%	0.115%
49	9.909	1443	1447	1451	rVB4	1834	2546	0.43%	0.048%
50	10.006	1457	1463	1466	rBV6	1191	2459	0.42%	0.046%
51	10.061	1466	1472	1478	rBV	279804	426490	72.24%	7.960%
52	10.201	1490	1495	1499	rBV	8499	12216	2.07%	0.228%
53	10.305	1501	1512	1518	rBV	65383	99964	16.93%	1.866%
54	10.360	1518	1521	1528	rVB3	6002	9225	1.56%	0.172%
55	10.592	1553	1559	1562	rBV5	1811	3153	0.53%	0.059%
56	10.646	1563	1568	1576	rVB	53730	70992	12.03%	1.325%
57	10.756	1580	1586	1587	rBV	4536	5436	0.92%	0.101%
58	10.860	1598	1603	1607	rBV4	5010	7662	1.30%	0.143%
59	10.963	1616	1620	1624	rBV	7381	10077	1.71%	0.188%
60	11.037	1630	1632	1636	rVB2	1424	1287	0.22%	0.024%
61	11.085	1636	1640	1641	rBV2	798	861	0.15%	0.016%
62	11.122	1642	1646	1651	rVB3	4804	6935	1.17%	0.129%
63	11.195	1653	1658	1669	rBV	206144	278731	47.21%	5.202%
64	11.305	1673	1676	1680	rBV	5945	7806	1.32%	0.146%
65	11.384	1685	1689	1695	rVB	11929	18838	3.19%	0.352%
66	11.457	1697	1701	1703	rBV	5257	7894	1.34%	0.147%
67	11.616	1723	1727	1733	rBV	10978	15007	2.54%	0.280%
68	11.713	1740	1743	1746	rBV	4370	5598	0.95%	0.104%
69	11.756	1746	1750	1759	rVB	30908	41159	6.97%	0.768%
70	11.847	1759	1765	1766	rBV4	1773	2378	0.40%	0.044%
71	11.896	1770	1773	1776	rVB	3418	3487	0.59%	0.065%
72	11.933	1777	1779	1783	rBV6	2230	3340	0.57%	0.062%
73	11.975	1784	1786	1789	rVB3	4315	4014	0.68%	0.075%
74	12.024	1789	1794	1800	rBV	362707	451225	76.43%	8.421%
75	12.091	1801	1805	1809	rBV	11344	14480	2.45%	0.270%
76	12.268	1827	1834	1837	rBV2	5396	8734	1.48%	0.163%

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 Misc : 2.78g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW9H3ME

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

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Peak separation: 5

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

77	12.323	1838	1843	1850	rVB	383734	467898	79.26%	8.732%
78	12.427	1856	1860	1864	rBV2	9147	10892	1.84%	0.203%
79	12.463	1864	1866	1872	rVB3	3806	5201	0.88%	0.097%
80	12.536	1874	1878	1880	rBV2	5694	7982	1.35%	0.149%
81	12.616	1888	1891	1894	rVB	3365	3745	0.63%	0.070%
82	12.847	1926	1929	1933	rVB2	2252	2415	0.41%	0.045%
83	12.969	1946	1949	1954	rVB3	5299	7654	1.30%	0.143%
84	13.042	1956	1961	1967	rBV9	1778	3990	0.68%	0.074%
85	13.268	1995	1998	2001	rBV	8189	10655	1.80%	0.199%
86	13.384	2014	2017	2021	rVB3	5384	6653	1.13%	0.124%
87	13.579	2045	2049	2055	rBV2	5518	8399	1.42%	0.157%
88	13.682	2063	2066	2068	rBV3	2007	2637	0.45%	0.049%
89	13.780	2078	2082	2088	rVB	17988	25409	4.30%	0.474%
90	13.847	2088	2093	2097	rVV	6080	8134	1.38%	0.152%
91	13.926	2100	2106	2113	rBV9	1139	3386	0.57%	0.063%
92	14.042	2121	2125	2128	rBV	10082	11482	1.94%	0.214%
93	14.109	2132	2136	2138	rBV2	3402	4653	0.79%	0.087%
94	14.640	2216	2223	2226	rBV2	16544	24225	4.10%	0.452%
95	14.755	2239	2242	2244	rBV2	8128	10372	1.76%	0.194%
96	14.780	2244	2246	2253	rVB	16304	21098	3.57%	0.394%
97	15.213	2314	2317	2324	rVB3	4068	5055	0.86%	0.094%
98	15.493	2358	2363	2368	rBV5	3666	6204	1.05%	0.116%
99	15.615	2379	2383	2386	rBV2	3372	4555	0.77%	0.085%
100	16.024	2449	2450	2454	rVB3	671	737	0.12%	0.014%

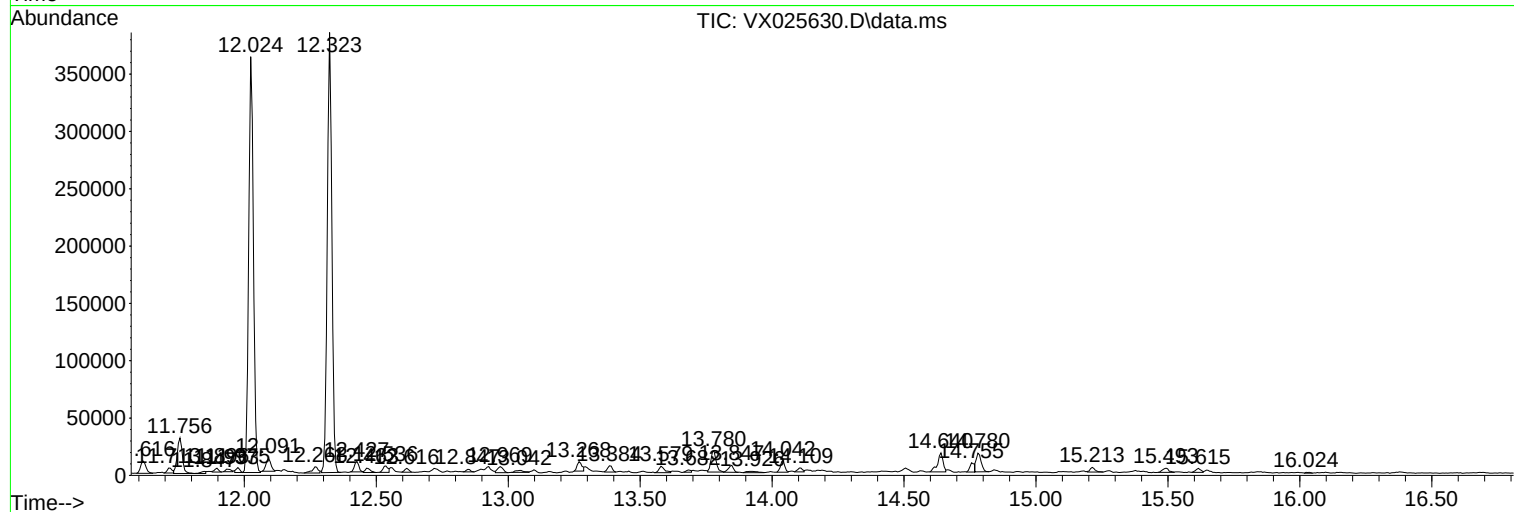
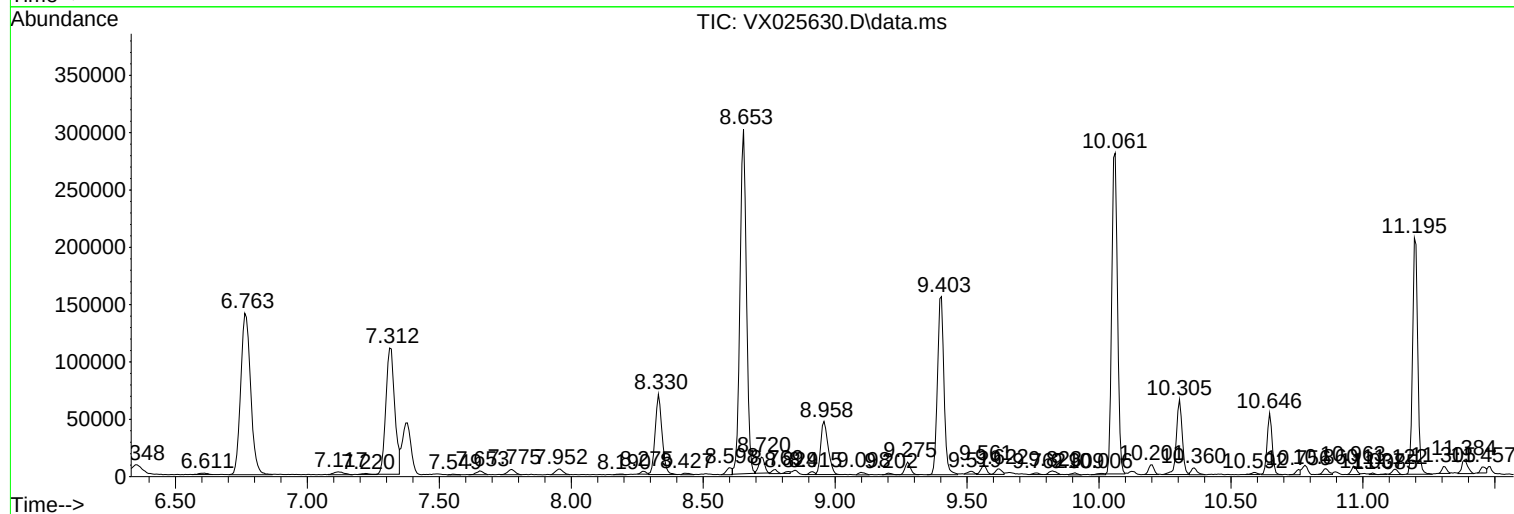
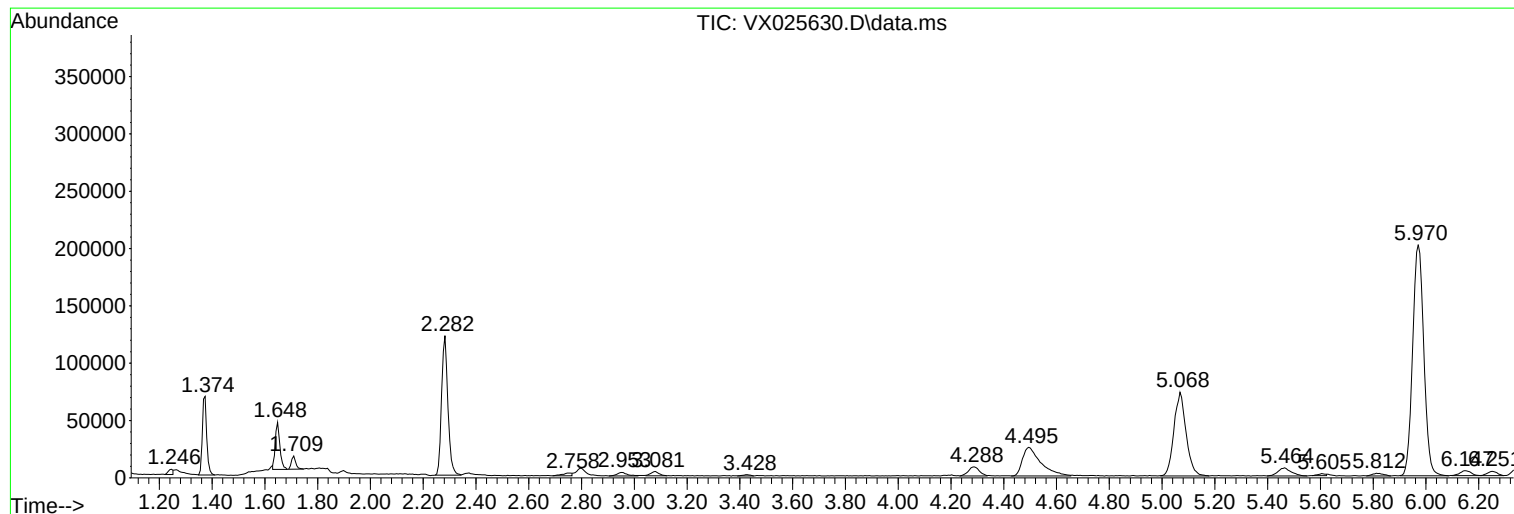
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Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025630.D
Acq On : 08 Dec 2021 19:30
Operator : JC/MD
Sample : M4883-17ME
Misc : 2.78g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9H3ME

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025630.D
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Operator : JC/MD
Sample : M4883-17ME
Misc : 2.78g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9H3ME

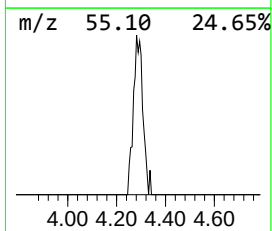
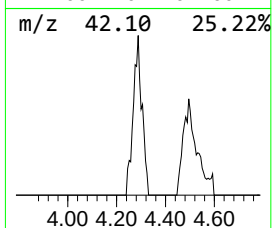
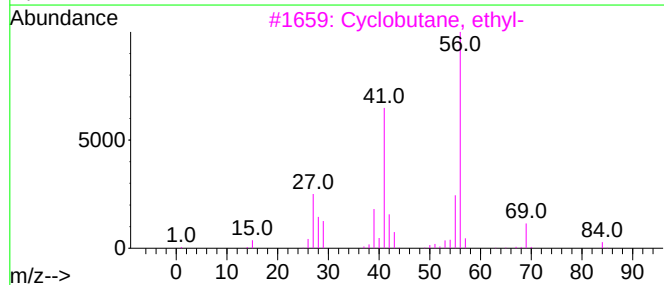
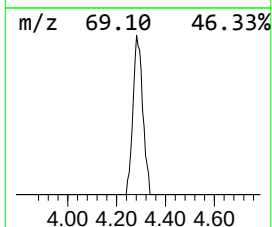
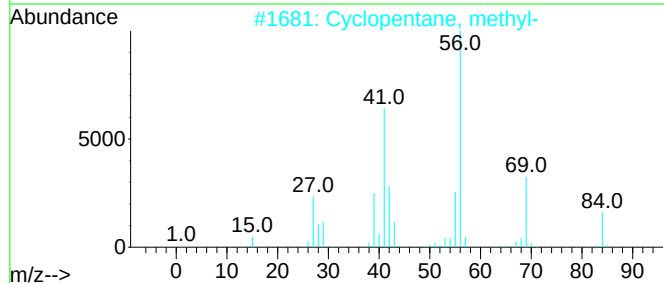
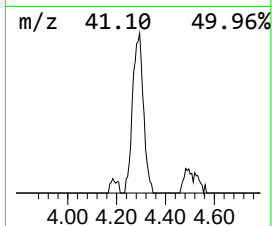
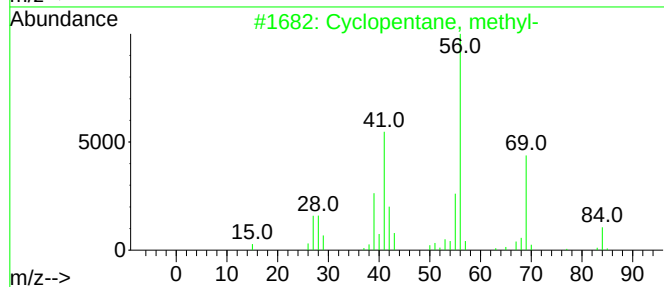
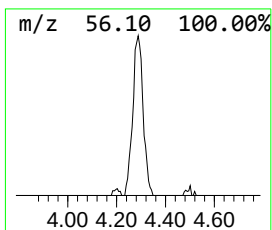
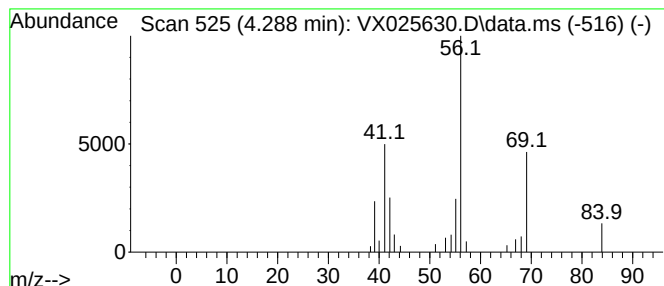
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Cyclic4.288 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.288	3.09 ug/L	22592	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	86
3			Cyclobutane, ethyl-	84	C6H12	004806-61-5	80
4			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
5			Cyclopentane, methyl-	84	C6H12	000096-37-7	78



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Operator : JC/MD
Sample : M4883-17ME
Misc : 2.78g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9H3ME

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

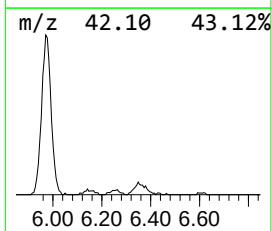
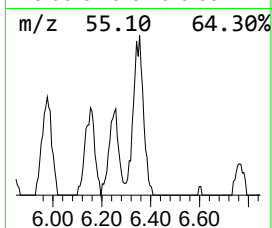
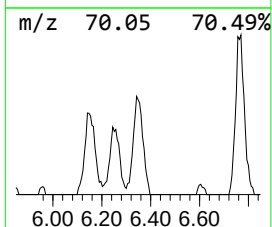
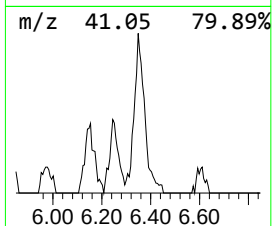
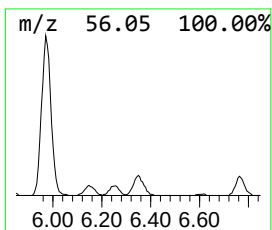
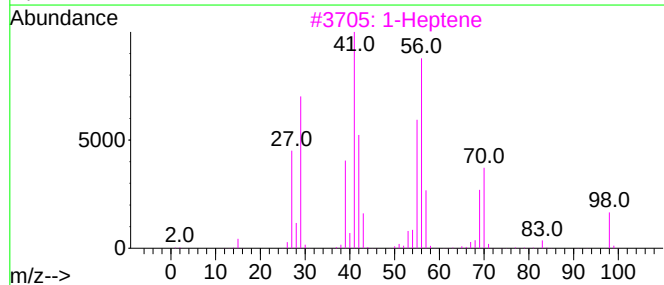
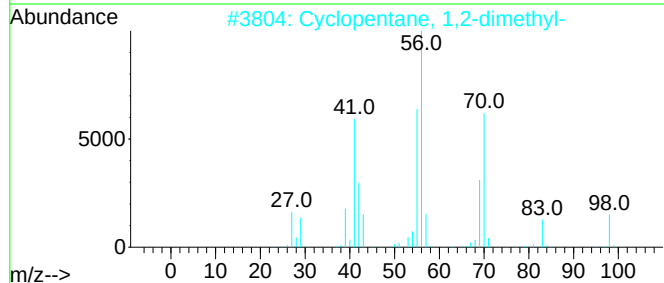
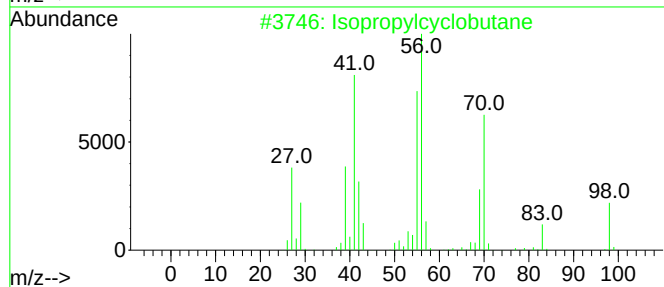
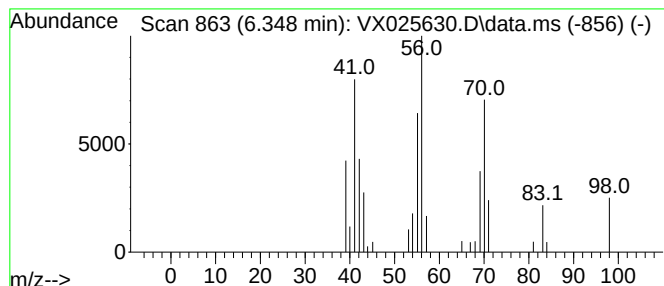
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 2 (DEL) Alkane: Cyclic6.348 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.348	3.37 ug/L	24648	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropylcyclobutane	98	C7H14	000872-56-0	81
2			Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	76
3			1-Heptene	98	C7H14	000592-76-7	62
4			(Z)-2-Heptene	98	C7H14	006443-92-1	60
5			Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	58



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Misc : 2.78g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9H3ME

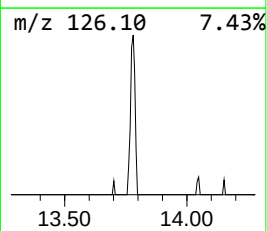
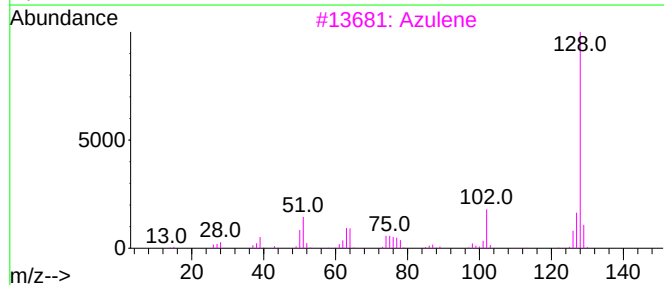
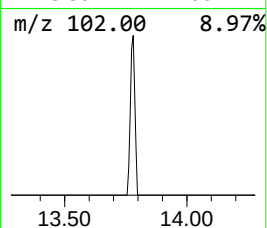
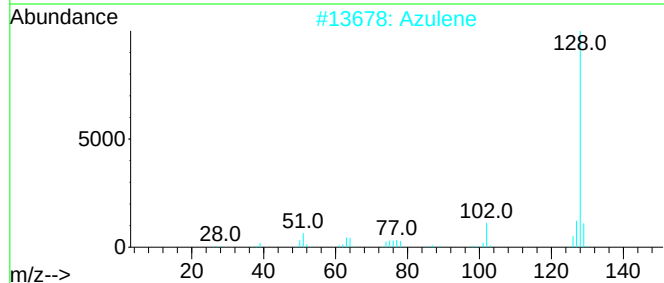
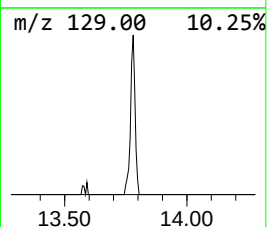
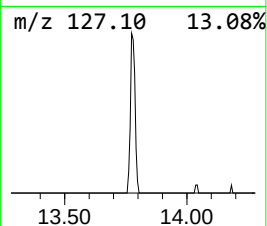
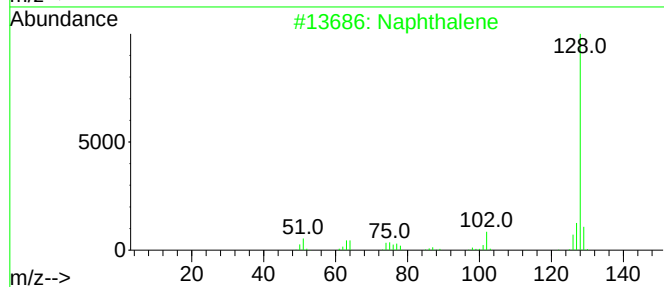
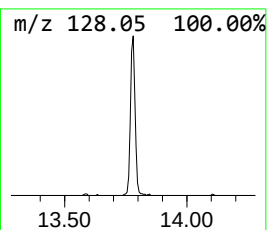
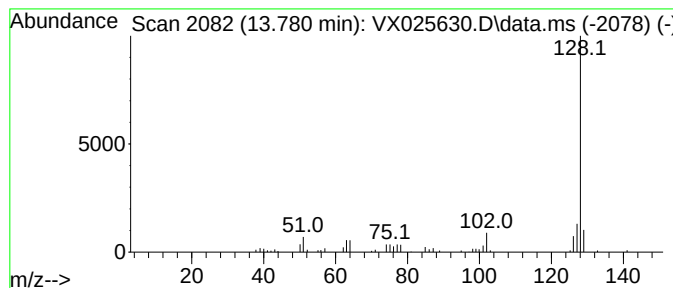
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Quant Title : VOC Analysis

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

Peak Number 4 Azulene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	2.82 ug/L	25409	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			Naphthalene	128	C10H8	000091-20-3	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025630.D
Acq On : 08 Dec 2021 19:30
Operator : JC/MD
Sample : M4883-17ME
Misc : 2.78g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9H3ME

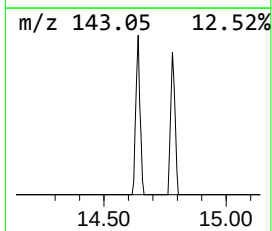
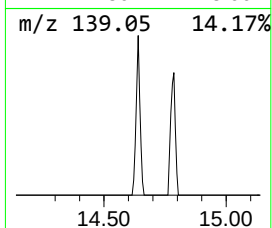
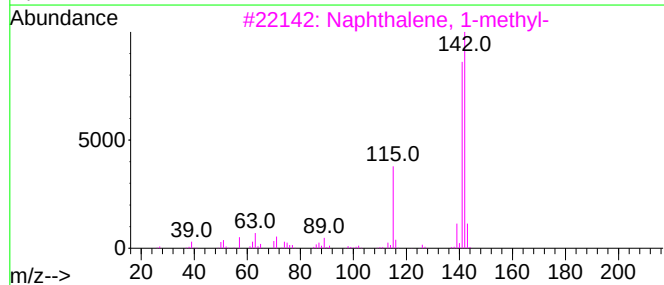
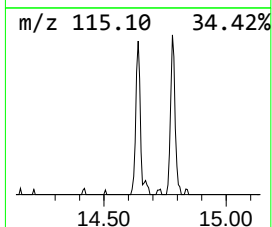
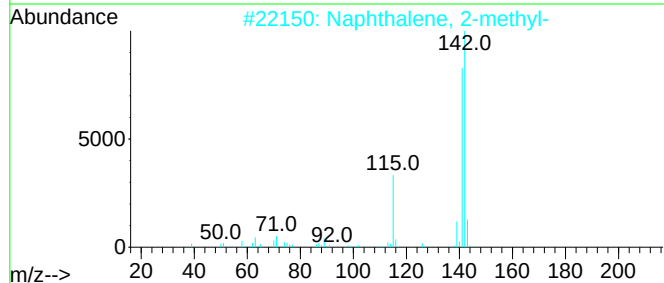
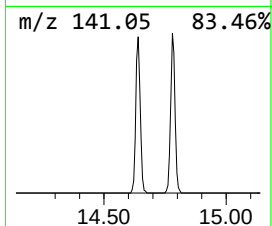
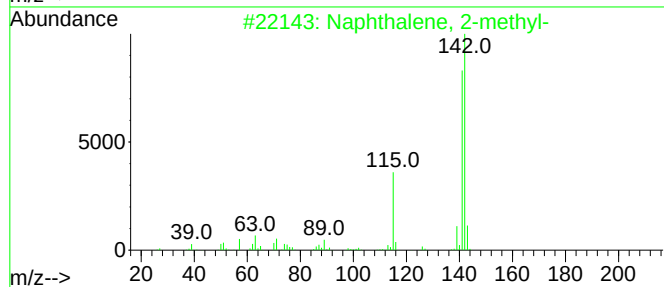
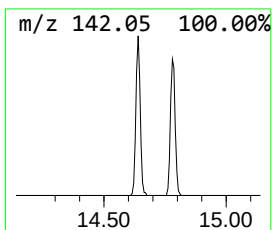
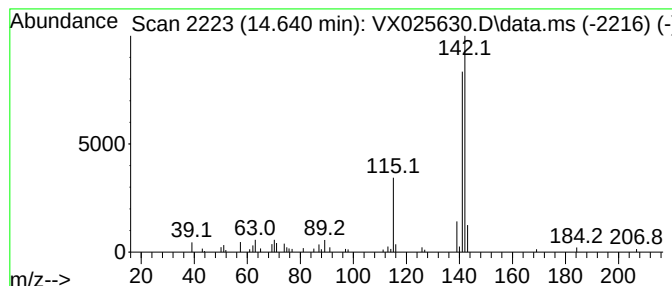
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML112221WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 Naphthalene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	2.68 ug/L	24225	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	95
2			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	95
3			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	95
4			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91
5			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120821\
Data File : VX025630.D
Acq On : 08 Dec 2021 19:30
Operator : JC/MD
Sample : M4883-17ME
Misc : 2.78g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EW9H3ME

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
(DEL) Alkane: C...	4.288	3.1	ug/L	22592	1	6.769	365670	50.0
(DEL) Alkane: C...	6.348	3.4	ug/L	24648	1	6.769	365670	50.0
Azulene	13.780	2.8	ug/L	25409	3	12.024	451225	50.0
Naphthalene, 2-...	14.640	2.7	ug/L	24225	3	12.024	451225	50.0