

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120721\
 Data File : VX025580.D
 Acq On : 07 Dec 2021 15:30
 Operator : JC/MD
 Sample : M4883-04ME
 Misc : 4.67g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EW9G0ME

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: VX025580.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	28	rBV	4196	6316	1.85%	0.206%
2	1.368	43	46	55	rVB	36323	40734	11.93%	1.331%
3	1.648	89	92	99	rVB	20908	24376	7.14%	0.796%
4	2.282	189	196	206	rBV	65906	110480	32.36%	3.609%
5	2.953	298	306	318	rBV	7667	21131	6.19%	0.690%
6	3.422	378	383	389	rVB3	514	1113	0.33%	0.036%
7	4.288	517	525	535	rVV5	2159	5771	1.69%	0.189%
8	4.495	548	559	592	rBV	15077	72074	21.11%	2.354%
9	4.721	592	596	597	rBV2	359	472	0.14%	0.015%
10	5.068	640	653	669	rBV	39666	135955	39.82%	4.441%
11	5.471	709	719	727	rVB5	1997	5986	1.75%	0.196%
12	5.812	770	775	783	rVB3	496	1141	0.33%	0.037%
13	5.971	789	801	824	rBV2	117922	341398	100.00%	11.152%
14	6.141	824	829	839	rVV6	1051	2738	0.80%	0.089%
15	6.251	842	847	854	rVB4	911	2063	0.60%	0.067%
16	6.361	854	865	880	rBV5	3202	11742	3.44%	0.384%
17	6.611	899	906	909	rVB5	461	865	0.25%	0.028%
18	6.763	921	931	947	rBV	89670	229349	67.18%	7.492%
19	7.123	982	990	1001	rBV	69843	158682	46.48%	5.183%
20	7.312	1013	1021	1028	rBV	65381	152268	44.60%	4.974%
21	7.653	1072	1077	1082	rVB4	933	1438	0.42%	0.047%
22	7.769	1091	1096	1101	rVB3	1048	1602	0.47%	0.052%
23	7.952	1121	1126	1131	rVB4	1376	2621	0.77%	0.086%
24	8.275	1174	1179	1182	rBV3	719	1185	0.35%	0.039%
25	8.330	1182	1188	1197	rVB	34783	63144	18.50%	2.063%
26	8.598	1227	1232	1233	rBV3	1804	2308	0.68%	0.075%
27	8.653	1234	1241	1248	rVV	168410	279221	81.79%	9.121%
28	8.720	1248	1252	1258	rVB	13729	21166	6.20%	0.691%
29	8.848	1270	1273	1277	rVB3	1088	1419	0.42%	0.046%
30	8.915	1280	1284	1286	rBV3	732	900	0.26%	0.029%
31	8.958	1286	1291	1299	rVV	22739	41871	12.26%	1.368%
32	9.104	1311	1315	1319	rBV3	580	834	0.24%	0.027%
33	9.275	1338	1343	1349	rVB	10759	16092	4.71%	0.526%
34	9.403	1357	1364	1375	rBV	92220	155771	45.63%	5.088%
35	9.561	1386	1390	1396	rVB2	2856	3910	1.15%	0.128%
36	9.616	1396	1399	1404	rBV2	2053	3342	0.98%	0.109%

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

37	9.708	1412	1414	1419	rVB2	540	805	0.24%	0.026%
38	9.763	1419	1423	1427	rBB3	313	384	0.11%	0.013%
39	9.830	1428	1434	1438	rVB3	977	1797	0.53%	0.059%
40	10.061	1466	1472	1479	rBV	175743	266488	78.06%	8.705%
41	10.195	1490	1494	1502	rVB	3684	4730	1.39%	0.155%
42	10.305	1502	1512	1517	rBV	11499	16980	4.97%	0.555%
43	10.360	1517	1521	1529	rVB4	1767	2438	0.71%	0.080%
44	10.586	1555	1558	1563	rBV4	597	948	0.28%	0.031%
45	10.646	1563	1568	1575	rVB	11119	14766	4.33%	0.482%
46	10.756	1582	1586	1588	rBV2	1098	1558	0.46%	0.051%
47	10.781	1588	1590	1593	rVB3	2181	2431	0.71%	0.079%
48	10.860	1597	1603	1606	rBV2	1796	2437	0.71%	0.080%
49	10.896	1606	1609	1614	rVB	1230	1758	0.51%	0.057%
50	10.964	1616	1620	1625	rVB	2964	4031	1.18%	0.132%
51	11.122	1642	1646	1651	rVB2	2169	3095	0.91%	0.101%
52	11.195	1653	1658	1667	rVB	123971	165772	48.56%	5.415%
53	11.274	1669	1671	1673	rVV2	362	441	0.13%	0.014%
54	11.311	1673	1677	1682	rVV	3580	5272	1.54%	0.172%
55	11.384	1686	1689	1694	rVV	3572	4962	1.45%	0.162%
56	11.457	1698	1701	1702	rVV	1549	1808	0.53%	0.059%
57	11.476	1702	1704	1713	rVB3	2782	3993	1.17%	0.130%
58	11.616	1723	1727	1731	rBV	2941	3331	0.98%	0.109%
59	11.713	1739	1743	1746	rBV3	1657	2236	0.65%	0.073%
60	11.756	1746	1750	1755	rVB2	8828	11497	3.37%	0.376%
61	11.848	1761	1765	1767	rBV2	561	802	0.23%	0.026%
62	11.890	1769	1772	1776	rVB3	1494	2164	0.63%	0.071%
63	11.939	1776	1780	1784	rBV5	1491	2473	0.72%	0.081%
64	11.976	1784	1786	1789	rVB2	969	878	0.26%	0.029%
65	12.024	1789	1794	1800	rBV	215860	267208	78.27%	8.729%
66	12.091	1802	1805	1809	rVB2	3133	3547	1.04%	0.116%
67	12.225	1822	1827	1830	rBV3	964	1592	0.47%	0.052%
68	12.268	1832	1834	1837	rVV2	1406	1691	0.50%	0.055%
69	12.323	1838	1843	1849	rVB	210358	261071	76.47%	8.528%
70	12.427	1855	1860	1863	rVB	3510	4022	1.18%	0.131%
71	12.469	1863	1867	1874	rVB4	1364	2248	0.66%	0.073%
72	12.536	1874	1878	1880	rBV2	1354	1774	0.52%	0.058%
73	12.731	1905	1910	1913	rBV4	755	1263	0.37%	0.041%
74	12.768	1913	1916	1919	rVV2	587	661	0.19%	0.022%
75	12.853	1926	1930	1933	rVB3	447	647	0.19%	0.021%
76	12.890	1933	1936	1939	rBV3	523	610	0.18%	0.020%

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 Title : VOC Analysis

77	12.927	1939	1942	1945	rBV2	915	1094	0.32%	0.036%
78	12.969	1945	1949	1957	rVB4	1356	2109	0.62%	0.069%
79	13.042	1960	1961	1964	rVV2	394	341	0.10%	0.011%
80	13.097	1968	1970	1973	rVB	543	384	0.11%	0.013%
81	13.219	1987	1990	1993	rBV3	419	399	0.12%	0.013%
82	13.268	1993	1998	2006	rBV2	3015	4852	1.42%	0.158%
83	13.384	2013	2017	2024	rBV4	1754	2539	0.74%	0.083%
84	13.579	2045	2049	2054	rBV2	1130	1460	0.43%	0.048%
85	13.634	2054	2058	2064	rVB4	558	793	0.23%	0.026%
86	13.780	2077	2082	2088	rVB	10230	13621	3.99%	0.445%
87	13.847	2089	2093	2096	rVB2	2174	2633	0.77%	0.086%
88	13.993	2114	2117	2119	rBV2	353	339	0.10%	0.011%
89	14.042	2120	2125	2128	rBV	2725	3279	0.96%	0.107%
90	14.103	2132	2135	2138	rBV2	801	925	0.27%	0.030%
91	14.506	2198	2201	2206	rVB5	854	1417	0.42%	0.046%
92	14.609	2215	2218	2219	rBV2	1185	977	0.29%	0.032%
93	14.640	2220	2223	2226	rVB	6641	6872	2.01%	0.224%
94	14.756	2239	2242	2244	rVV2	2323	3015	0.88%	0.098%
95	14.780	2244	2246	2251	rVV	7519	8985	2.63%	0.294%
96	14.847	2254	2257	2261	rVB4	745	898	0.26%	0.029%
97	15.213	2314	2317	2322	rVB4	1346	1918	0.56%	0.063%
98	15.268	2324	2326	2330	rVB4	389	455	0.13%	0.015%
99	15.487	2357	2362	2366	rBV5	1021	1693	0.50%	0.055%
100	15.615	2378	2383	2387	rBV2	1434	2221	0.65%	0.073%

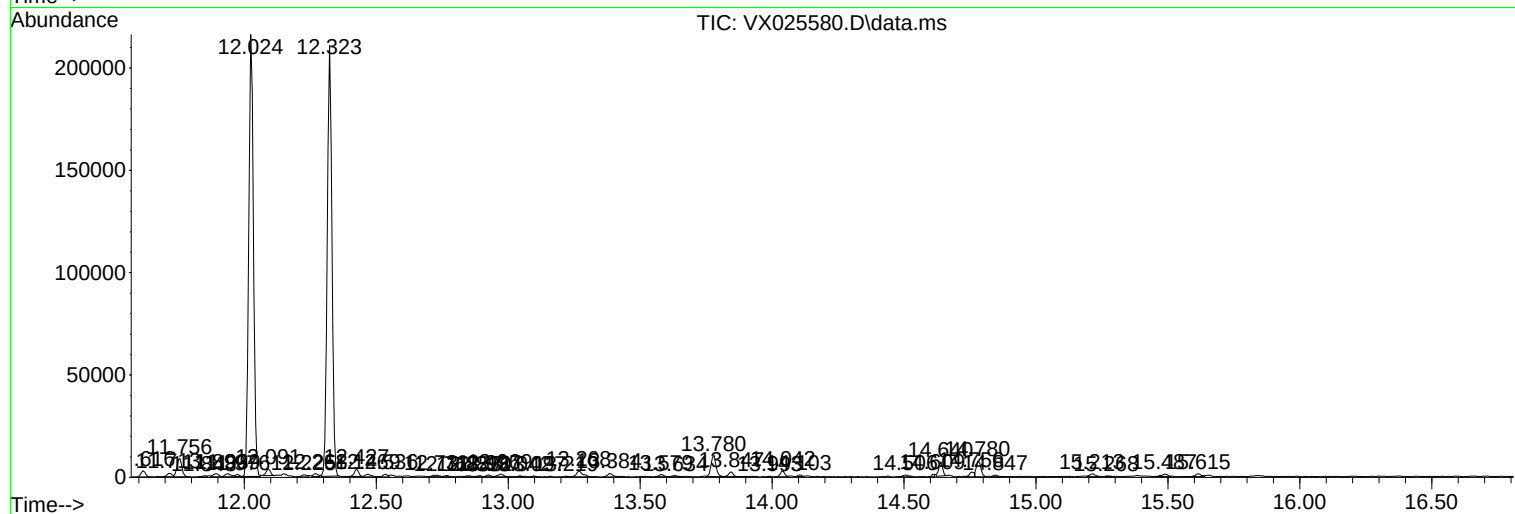
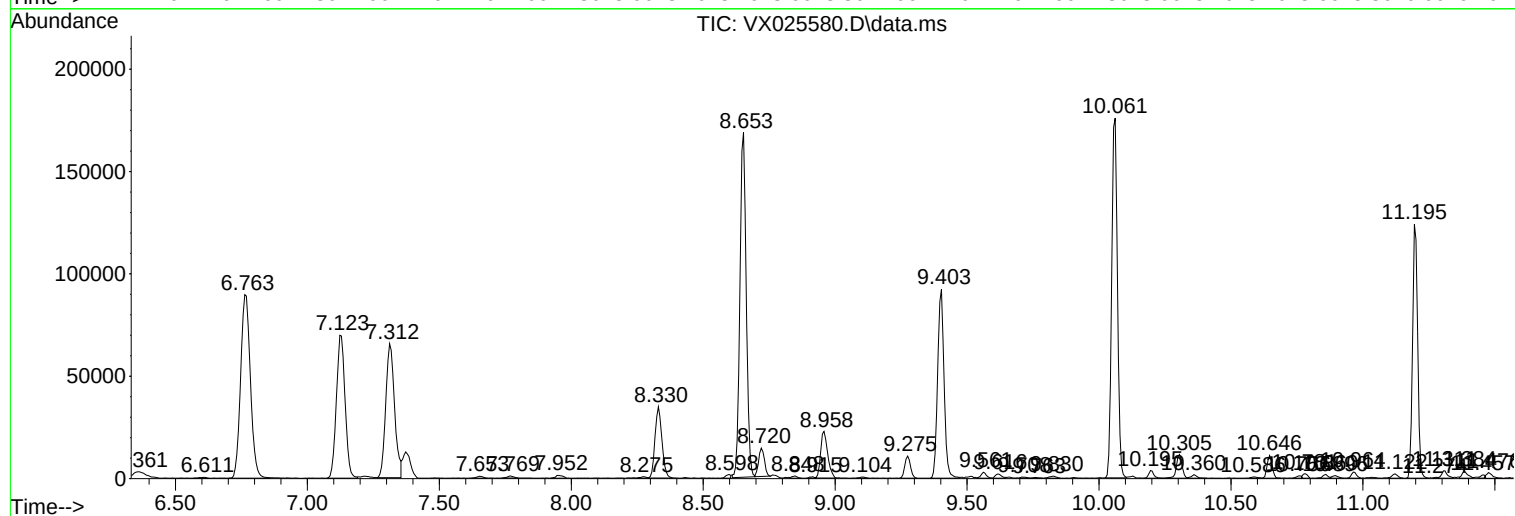
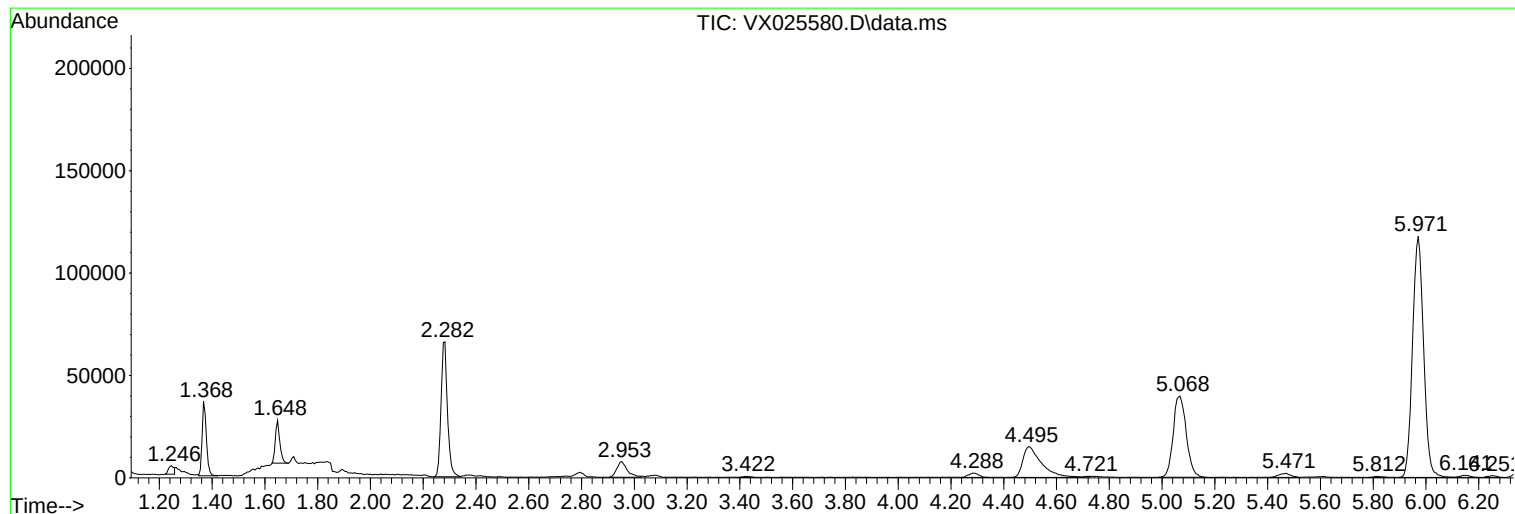
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 16 Sample Multiplier: 1

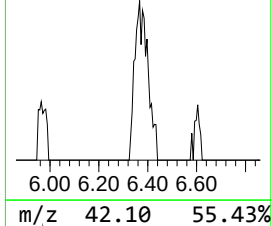
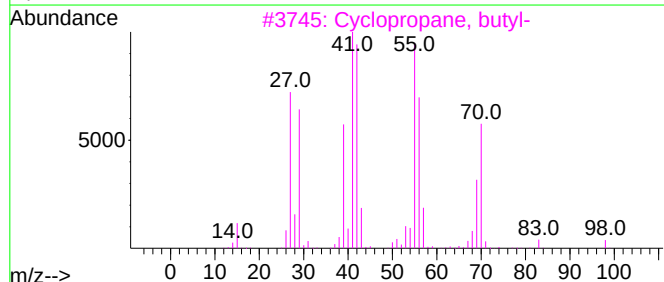
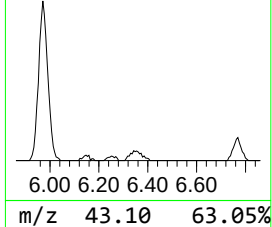
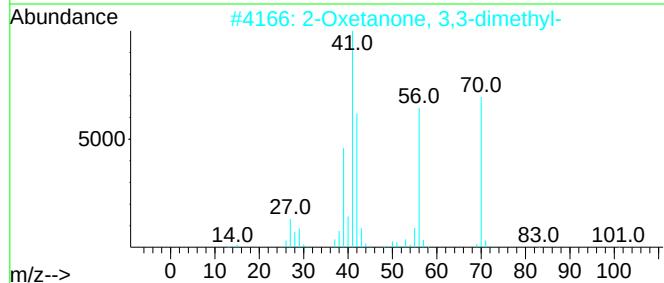
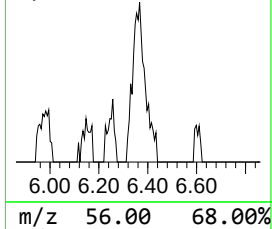
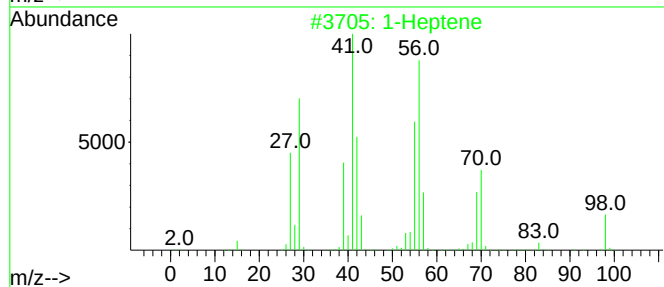
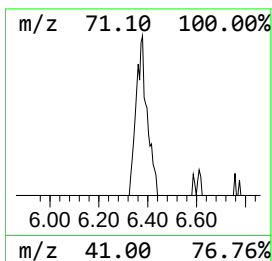
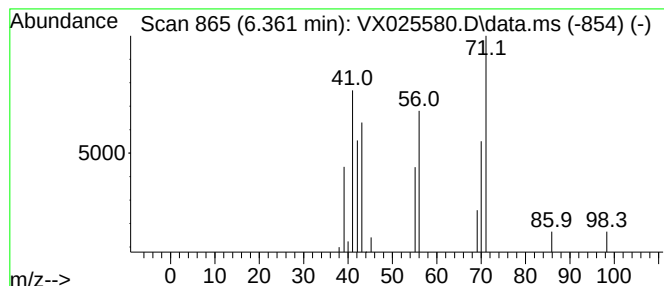
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MSVOA_X
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
6.361	2.56 ug/L	11742	1,4-Difluorobenzene	6.763	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptene	98	C7H14	000592-76-7	49
2	2-Oxetanone, 3,3-dimethyl-	100	C5H8O2	001955-45-9	47
3	Cyclopropane, butyl-	98	C7H14	000930-57-4	47
4	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	38
5	1-Hexene	84	C6H12	000592-41-6	38



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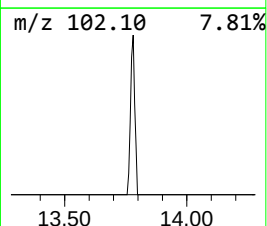
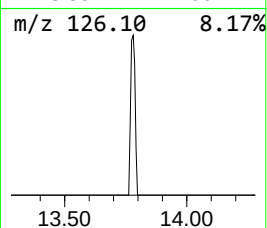
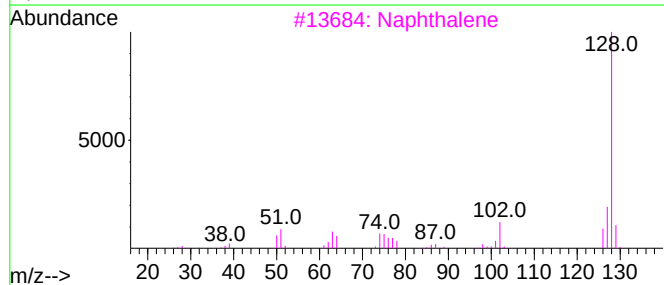
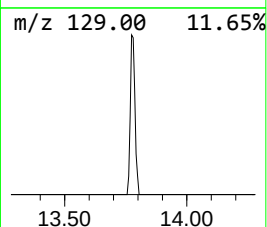
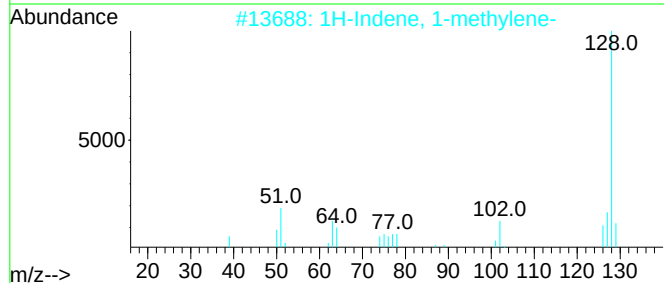
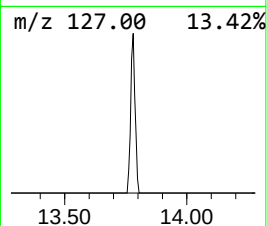
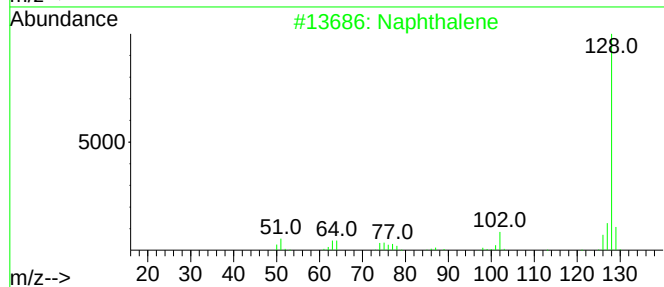
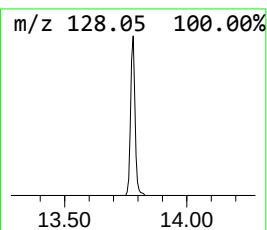
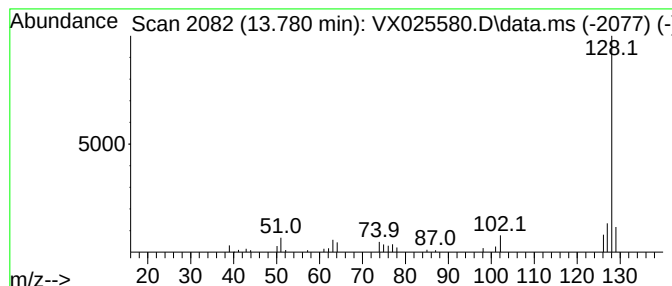
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Azulene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.780	2.55 ug/L	13621	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	94
2			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	91
3			Naphthalene	128	C10H8	000091-20-3	91
4			Azulene	128	C10H8	000275-51-4	91
5			Azulene	128	C10H8	000275-51-4	91



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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: S...	6.361	2.6	ug/L	11742	1	6.763	229349	50.0
Azulene	13.780	2.5	ug/L	13621	3	12.024	267208	50.0