

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041823\
 Data File : VX035146.D
 Acq On : 19 Apr 2023 00:34
 Operator : JC/MD
 Sample : 02397-10
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMM2

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\SFAMXML041823WMA.M
 Title : VOC Analysis

Signal : TIC: VX035146.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	17	rVB	30373	29119	0.01%	0.004%
2	1.264	25	29	31	rBV	8202	8354	0.00%	0.001%
3	1.294	31	34	42	rVV	14652	33426	0.02%	0.005%
4	1.367	42	46	54	rVB	258201	280986	0.14%	0.039%
5	1.495	64	67	71	rVB	3889	4148	0.00%	0.001%
6	1.599	81	84	85	rBV3	1020	929	0.00%	0.000%
7	1.672	91	96	105	rBV	179571	237263	0.12%	0.033%
8	1.751	105	109	114	rVB	11219	16135	0.01%	0.002%
9	1.910	131	135	138	rVV	7527	10669	0.01%	0.001%
10	1.959	138	143	149	rVB2	10689	16314	0.01%	0.002%
11	2.068	158	161	165	rBV2	4194	4958	0.00%	0.001%
12	2.160	173	176	184	rVB5	4281	7712	0.00%	0.001%
13	2.306	194	200	210	rBV	448070	706832	0.36%	0.098%
14	2.385	210	213	224	rVB2	3377	8192	0.00%	0.001%
15	2.513	229	234	236	rBV3	783	1155	0.00%	0.000%
16	2.727	262	269	272	rBV6	2041	4859	0.00%	0.001%
17	2.782	273	278	281	rBV5	4888	8842	0.00%	0.001%
18	2.824	281	285	290	rVV	10480	17937	0.01%	0.002%
19	2.989	307	312	314	rVV4	533	804	0.00%	0.000%
20	3.099	323	330	341	rVB	14495	33040	0.02%	0.005%
21	3.336	360	369	375	rBB6	1867	3909	0.00%	0.001%
22	3.452	379	388	395	rBV	10559	24802	0.01%	0.003%
23	3.666	415	423	431	rVB7	1217	3321	0.00%	0.000%
24	3.946	464	469	476	rVB	967	2033	0.00%	0.000%
25	4.306	516	528	543	rVB	163693	469408	0.24%	0.065%
26	4.458	544	553	569	rBV	125507	370573	0.19%	0.051%
27	5.056	638	651	672	rBV2	245709	767528	0.39%	0.106%
28	5.470	708	719	734	rVV	62040	196123	0.10%	0.027%
29	5.623	737	744	745	rVV6	2461	4458	0.00%	0.001%
30	5.677	745	753	766	rVB2	12634	40328	0.02%	0.006%
31	5.836	769	779	789	rBV6	7094	23759	0.01%	0.003%
32	5.976	789	802	803	rBV2	661376	1493757	0.76%	0.207%
33	6.049	803	814	841	rVV	16299688	46897296	23.84%	6.505%
34	6.263	843	849	856	rVV8	10171	32346	0.02%	0.004%
35	6.360	857	865	875	rVV5	11463	35363	0.02%	0.005%
36	6.458	879	881	883	rVV3	1026	1023	0.00%	0.000%

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 Title : VOC Analysis

37	6.482	883	885	891	rVV5	645	842	0.00%	0.000%
38	6.610	902	906	914	rVB6	2617	5361	0.00%	0.001%
39	6.763	918	931	947	rBV	463799	1111953	0.57%	0.154%
40	7.116	984	989	996	rVB7	2314	5442	0.00%	0.001%
41	7.311	1011	1021	1028	rBV	397236	919281	0.47%	0.128%
42	7.488	1045	1050	1054	rVV4	1260	1870	0.00%	0.000%
43	7.659	1071	1078	1086	rVB2	9178	18282	0.01%	0.003%
44	7.945	1122	1125	1127	rBV2	1101	1456	0.00%	0.000%
45	8.110	1145	1152	1157	rBV4	3131	6051	0.00%	0.001%
46	8.323	1181	1187	1200	rBV	253845	421958	0.21%	0.059%
47	8.409	1200	1201	1202	rVV	1478	925	0.00%	0.000%
48	8.433	1202	1205	1209	rVV6	1364	2332	0.00%	0.000%
49	8.506	1211	1217	1226	rVB8	1188	4255	0.00%	0.001%
50	8.646	1234	1240	1248	rVV	1026860	1655609	0.84%	0.230%
51	8.720	1248	1252	1266	rVV	40691	69493	0.04%	0.010%
52	8.951	1284	1290	1303	rVV	186256	275322	0.14%	0.038%
53	9.274	1334	1343	1351	rBV2	11858	18287	0.01%	0.003%
54	9.390	1356	1362	1380	rBV	544063	846131	0.43%	0.117%
55	10.116	1465	1481	1484	rBV4	57254856	196725608	100.00%	27.287%
56	10.305	1509	1512	1515	rBV	11867	17235	0.01%	0.002%
57	10.646	1564	1568	1576	rVB2	9581	17000	0.01%	0.002%
58	10.762	1585	1587	1590	rBV3	1028	1006	0.00%	0.000%
59	10.963	1616	1620	1625	rBV3	3310	4502	0.00%	0.001%
60	11.091	1639	1641	1644	rVB4	1151	1164	0.00%	0.000%
61	11.122	1644	1646	1649	rVB4	979	1082	0.00%	0.000%
62	11.195	1652	1658	1671	rVV2	728566	984674	0.50%	0.137%
63	11.311	1673	1677	1679	rVV4	1729	2307	0.00%	0.000%
64	11.365	1681	1686	1692	rVV	133810	171451	0.09%	0.024%
65	11.420	1692	1695	1697	rVV2	7409	9404	0.00%	0.001%
66	11.457	1697	1701	1708	rVV	53475	72892	0.04%	0.010%
67	11.707	1740	1742	1745	rVB4	1360	1412	0.00%	0.000%
68	11.762	1745	1751	1756	rBV4	2235	3985	0.00%	0.001%
69	11.975	1780	1786	1792	rBV	26883642	41133427	20.91%	5.705%
70	12.067	1792	1801	1806	rVB2	60930752	136393858	69.33%	18.918%
71	12.225	1825	1827	1829	rVB2	3795	2862	0.00%	0.000%
72	12.377	1839	1852	1856	rBV3	62684010	179094292	91.04%	24.841%
73	12.707	1901	1906	1910	rVB3	11951	18613	0.01%	0.003%
74	12.877	1929	1934	1936	rBV6	6951	10592	0.01%	0.001%
75	12.920	1936	1941	1952	rVB	384662	491863	0.25%	0.068%
76	13.060	1958	1964	1969	rBV	83381	157137	0.08%	0.022%

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 Title : VOC Analysis

77	13.115	1969	1973	1980	rVB	68380	88028	0.04%	0.012%
78	13.194	1981	1986	1999	rVB	200832	268943	0.14%	0.037%
79	13.347	2009	2011	2013	rVB3	1050	975	0.00%	0.000%
80	13.383	2013	2017	2023	rBV	22684	31289	0.02%	0.004%
81	13.603	2045	2053	2058	rBV	47933498	75346041	38.30%	10.451%
82	13.780	2077	2082	2088	rVB	41762	56066	0.03%	0.008%
83	13.963	2106	2112	2118	rBV	20911260	28526076	14.50%	3.957%
84	14.164	2143	2145	2150	rVB5	3547	4363	0.00%	0.001%
85	14.316	2169	2170	2172	rBV2	1141	802	0.00%	0.000%
86	14.334	2172	2173	2175	rVV	1751	1642	0.00%	0.000%
87	14.377	2175	2180	2186	rVB5	11954	22571	0.01%	0.003%
88	14.487	2195	2198	2200	rBV3	827	805	0.00%	0.000%
89	14.542	2203	2207	2210	rBV4	4664	5596	0.00%	0.001%
90	14.633	2217	2222	2230	rVB4	10374	18393	0.01%	0.003%
91	14.786	2236	2247	2254	rBV	944791	1330085	0.68%	0.184%
92	14.926	2265	2270	2273	rBV7	2510	4028	0.00%	0.001%
93	15.200	2313	2315	2316	rVV2	1556	1405	0.00%	0.000%
94	15.249	2317	2323	2336	rVV	2005220	2736214	1.39%	0.380%
95	15.340	2336	2338	2340	rVV3	1790	1716	0.00%	0.000%
96	15.846	2419	2421	2425	rBV4	781	1097	0.00%	0.000%
97	15.907	2428	2431	2433	rVB4	1134	1075	0.00%	0.000%
98	16.035	2449	2452	2454	rVB4	832	783	0.00%	0.000%
99	16.127	2466	2467	2470	rBV3	857	921	0.00%	0.000%
100	16.505	2524	2529	2539	rVB3	16682	31984	0.02%	0.004%

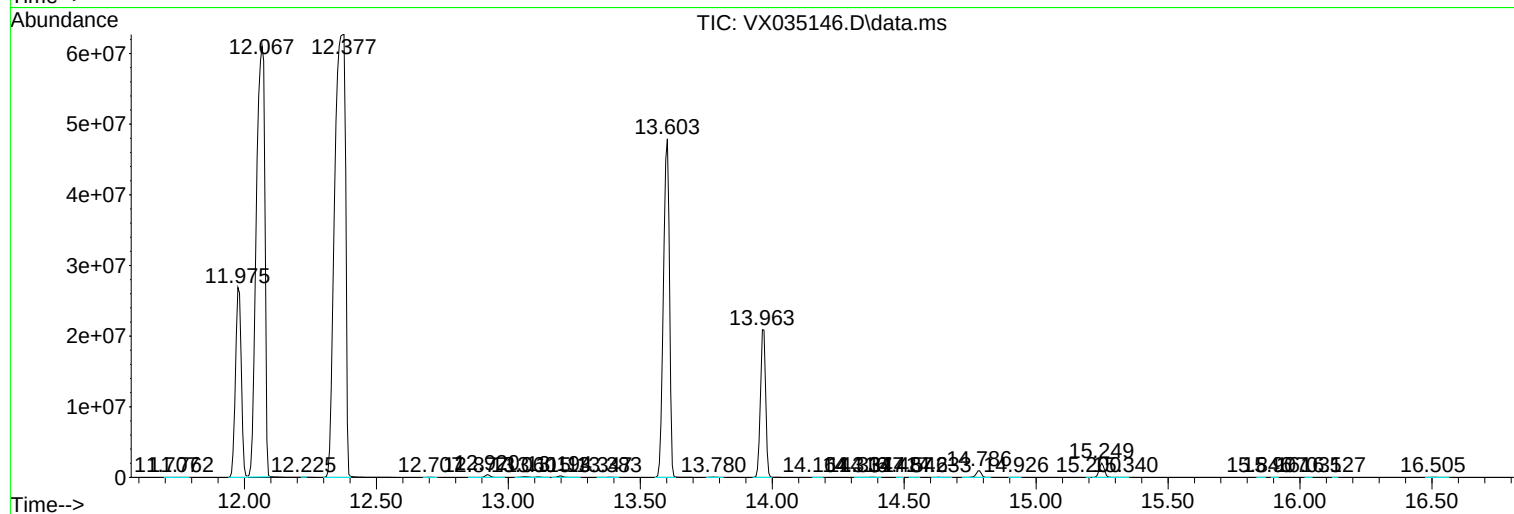
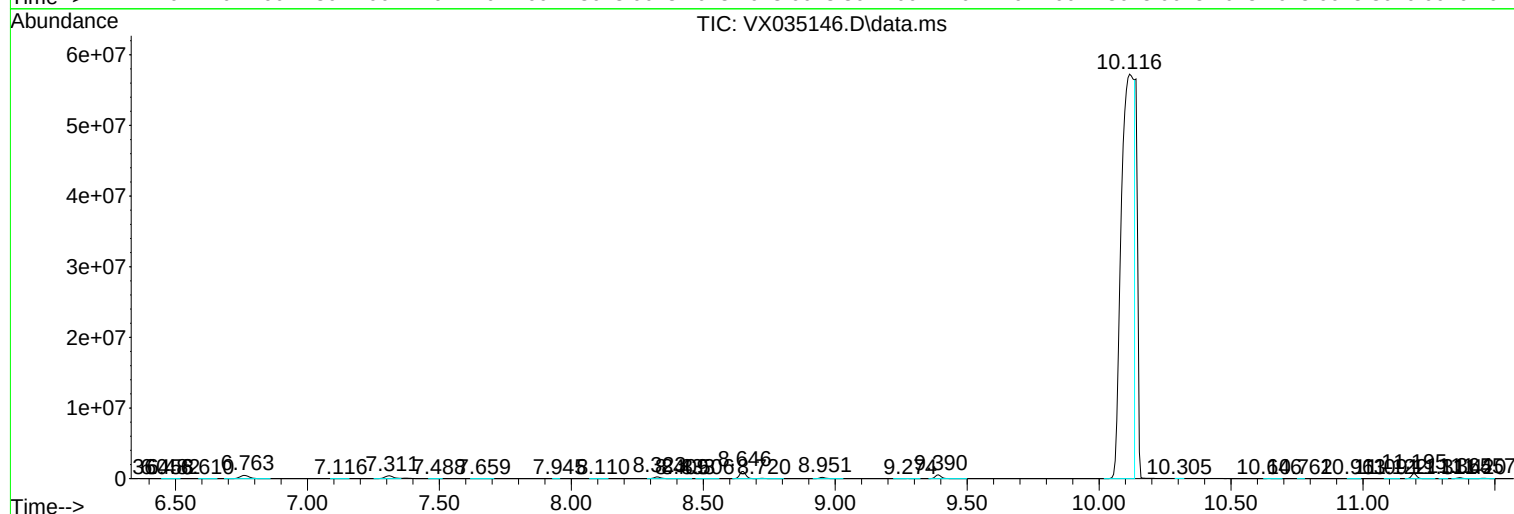
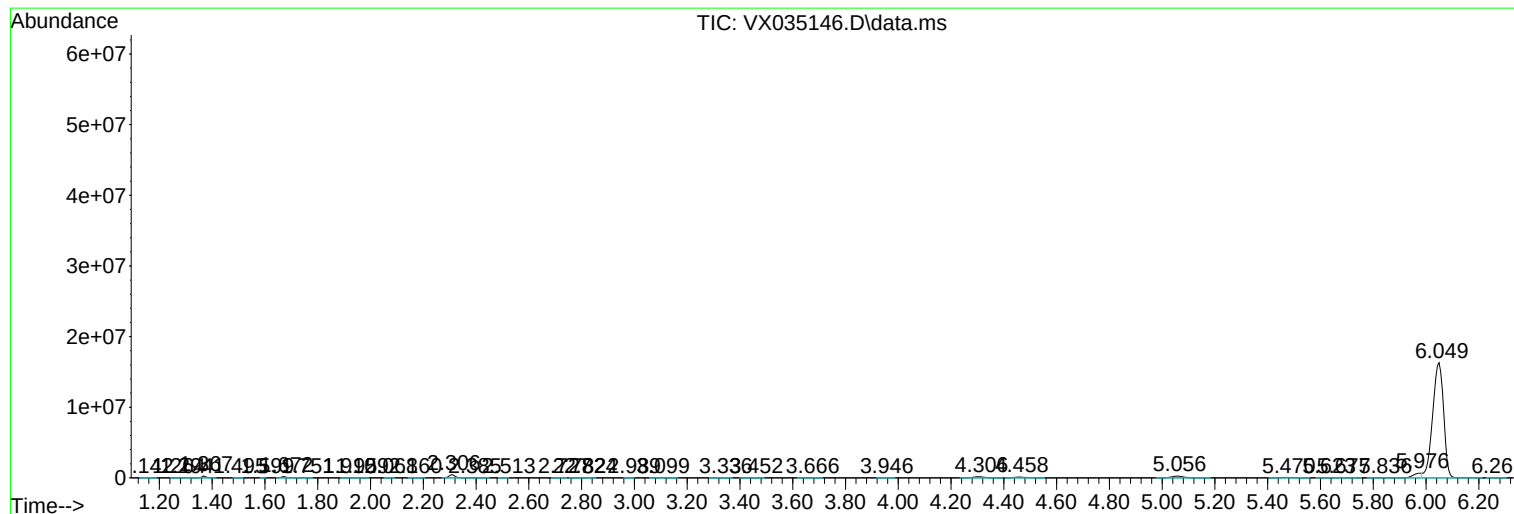
Sum of corrected areas: 720959815

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VO41823\
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Acq On : 19 Apr 2023 00:34
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
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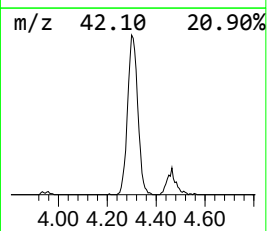
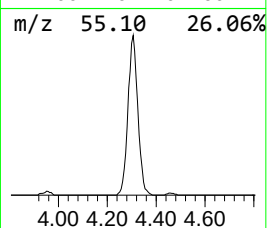
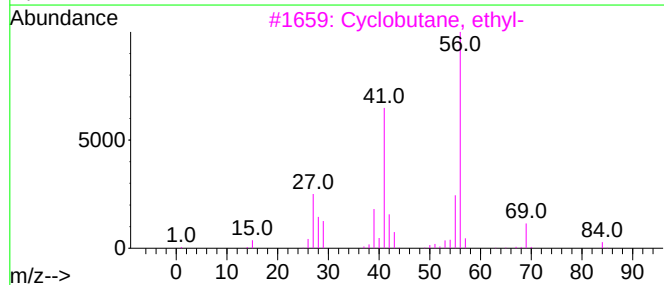
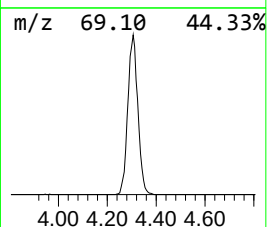
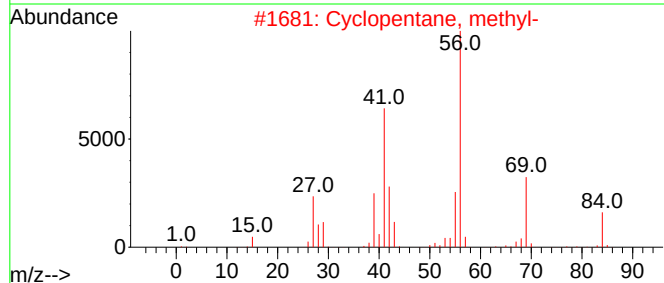
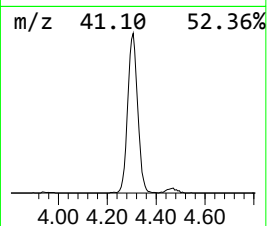
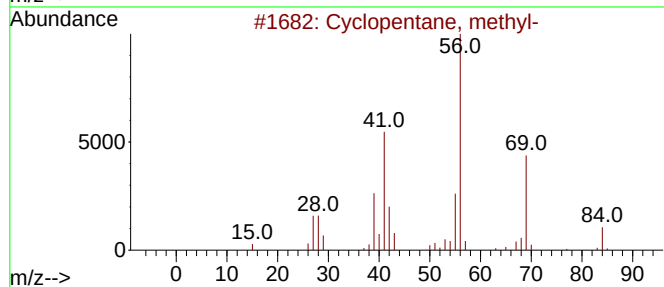
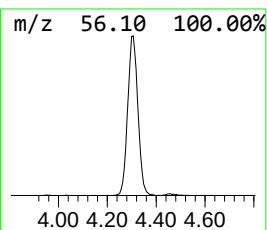
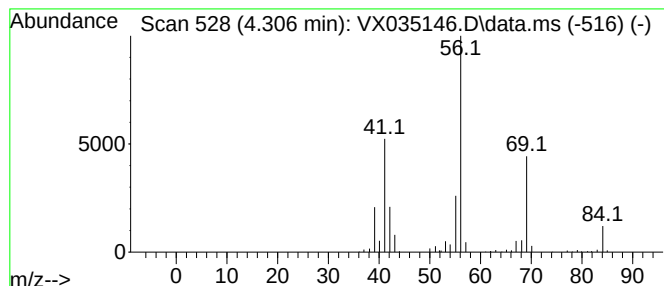
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041823WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Cyclic4.306 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	21.11 ug/L	469408	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
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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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: C...	4.306	21.1	ug/L	469408	1	6.763	1111950	50.0