

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041124\
 Data File : VX040973.D
 Acq On : 11 Apr 2024 12:50
 Operator : JC/MD
 Sample : P2048-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MC0R47

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\SFAMXML041024WMA.M
 Title : VOC Analysis

Signal : TIC: VX040973.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	33	rBV	8900	18787	0.01%	0.005%
2	1.368	42	46	57	rBV	142178	156404	0.09%	0.042%
3	1.666	91	95	106	rBV	100505	150942	0.09%	0.041%
4	2.307	194	200	209	rBV	247318	401015	0.23%	0.109%
5	2.374	209	211	220	rVB	2295	3903	0.00%	0.001%
6	2.477	220	228	229	rBV3	500	1078	0.00%	0.000%
7	2.514	231	234	241	rVB3	1351	1927	0.00%	0.001%
8	2.788	274	279	283	rVV	656	1373	0.00%	0.000%
9	2.861	285	291	300	rVV	8663	18314	0.01%	0.005%
10	2.934	300	303	305	rVV	400	515	0.00%	0.000%
11	2.953	305	306	307	rVV	505	305	0.00%	0.000%
12	3.093	322	329	336	rBV6	2398	5501	0.00%	0.001%
13	3.434	383	385	386	rBV2	256	229	0.00%	0.000%
14	3.447	386	387	391	rVV2	355	309	0.00%	0.000%
15	3.611	410	414	417	rVV2	414	651	0.00%	0.000%
16	3.825	447	449	453	rVB2	249	302	0.00%	0.000%
17	3.867	453	456	459	rBV2	228	308	0.00%	0.000%
18	4.306	518	528	538	rBV2	20859	59979	0.03%	0.016%
19	4.459	543	553	583	rBV2	68305	240387	0.14%	0.065%
20	4.654	583	585	586	rVB	351	207	0.00%	0.000%
21	5.056	638	651	669	rBV	139309	439858	0.25%	0.119%
22	5.221	677	678	684	rVB3	544	734	0.00%	0.000%
23	5.391	699	706	708	rBV4	895	1849	0.00%	0.001%
24	5.477	710	720	729	rVB4	8059	23772	0.01%	0.006%
25	5.568	729	735	736	rBV	1098	1502	0.00%	0.000%
26	5.690	752	755	758	rBV	247	220	0.00%	0.000%
27	5.782	767	770	772	rBV	270	286	0.00%	0.000%
28	6.105	787	823	857	rBV2	36775203	173149079	100.00%	46.849%
29	6.763	922	931	948	rVB	285099	670059	0.39%	0.181%
30	7.001	966	970	973	rBV4	405	554	0.00%	0.000%
31	7.129	984	991	1001	rVB5	7561	18267	0.01%	0.005%
32	7.239	1007	1009	1012	rBV2	297	354	0.00%	0.000%
33	7.312	1012	1021	1039	rVV	214865	486925	0.28%	0.132%
34	7.470	1045	1047	1050	rBV3	453	632	0.00%	0.000%
35	7.550	1059	1060	1064	rVB2	242	249	0.00%	0.000%
36	7.671	1076	1080	1088	rVV5	1685	3762	0.00%	0.001%

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 Title : VOC Analysis

37	7.787	1098	1099	1101	rVB2	377	253	0.00%	0.000%
38	7.927	1120	1122	1123	rBV	347	207	0.00%	0.000%
39	7.940	1123	1124	1126	rBV2	782	644	0.00%	0.000%
40	8.116	1149	1153	1157	rVB4	1042	1642	0.00%	0.000%
41	8.251	1173	1175	1176	rBV	410	271	0.00%	0.000%
42	8.324	1181	1187	1203	rBV	151138	247261	0.14%	0.067%
43	8.494	1213	1215	1218	rBV2	474	599	0.00%	0.000%
44	8.574	1226	1228	1233	rVB3	636	906	0.00%	0.000%
45	8.647	1234	1240	1249	rVV	573155	923961	0.53%	0.250%
46	8.720	1250	1252	1260	rVB2	6431	10647	0.01%	0.003%
47	8.848	1271	1273	1274	rVB	446	251	0.00%	0.000%
48	8.952	1284	1290	1301	rBV	109339	164620	0.10%	0.045%
49	9.275	1336	1343	1349	rBV	5987	8801	0.01%	0.002%
50	9.385	1356	1361	1381	rBV2	306026	490317	0.28%	0.133%
51	9.537	1382	1386	1392	rVB5	1517	3164	0.00%	0.001%
52	9.610	1397	1398	1403	rVB3	575	534	0.00%	0.000%
53	9.848	1435	1437	1441	rVB3	368	507	0.00%	0.000%
54	10.110	1465	1480	1485	rBV2	42955025	115262753	66.57%	31.187%
55	10.647	1565	1568	1577	rVB6	1528	3032	0.00%	0.001%
56	10.927	1612	1614	1616	rBV2	390	359	0.00%	0.000%
57	10.964	1617	1620	1623	rVV3	795	1113	0.00%	0.000%
58	11.037	1630	1632	1635	rVB3	411	361	0.00%	0.000%
59	11.092	1636	1641	1649	rVB	4533	6882	0.00%	0.002%
60	11.189	1652	1657	1672	rVB	400700	528045	0.30%	0.143%
61	11.311	1672	1677	1682	rBV	8726	12630	0.01%	0.003%
62	11.366	1682	1686	1692	rVB	8859	12051	0.01%	0.003%
63	11.421	1692	1695	1697	rBV	468	407	0.00%	0.000%
64	11.457	1697	1701	1706	rBV	5407	7311	0.00%	0.002%
65	11.713	1742	1743	1747	rVV2	534	435	0.00%	0.000%
66	11.756	1747	1750	1756	rVV5	1050	1239	0.00%	0.000%
67	11.829	1760	1762	1765	rVB2	209	228	0.00%	0.000%
68	11.866	1765	1768	1770	rBV	215	307	0.00%	0.000%
69	11.969	1779	1785	1790	rBV	2302680	2817029	1.63%	0.762%
70	12.049	1790	1798	1803	rBV	34005945	45668676	26.38%	12.357%
71	12.341	1837	1846	1851	rBV	19967704	26485627	15.30%	7.166%
72	12.622	1890	1892	1894	rBV2	419	272	0.00%	0.000%
73	12.701	1901	1905	1908	rBV4	490	902	0.00%	0.000%
74	12.768	1910	1916	1920	rBV4	2299	3455	0.00%	0.001%
75	12.927	1936	1942	1949	rVB3	4859	7319	0.00%	0.002%
76	13.067	1961	1965	1968	rVB3	1465	2369	0.00%	0.001%

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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 0 % of largest Peak

Max Peaks: 100

Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041024WMA.M
Title : VOC Analysis

77	13.116	1969	1973	1976	rBV3	1865	2049	0.00%	0.001%
78	13.256	1994	1996	1998	rBV	211	263	0.00%	0.000%
79	13.298	2001	2003	2008	rVB3	293	308	0.00%	0.000%
80	13.347	2010	2011	2015	rVB2	215	218	0.00%	0.000%
81	13.487	2033	2034	2039	rVB	320	240	0.00%	0.000%
82	13.585	2045	2050	2062	rBV	832220	1026186	0.59%	0.278%
83	13.780	2077	2082	2090	rVB2	4105	6040	0.00%	0.002%
84	13.963	2107	2112	2117	rBV2	1642	2300	0.00%	0.001%
85	14.128	2135	2139	2143	rVB2	2750	3913	0.00%	0.001%
86	14.609	2216	2218	2220	rVV2	322	242	0.00%	0.000%
87	14.676	2226	2229	2231	rVB2	200	221	0.00%	0.000%
88	14.804	2248	2250	2253	rVV3	329	288	0.00%	0.000%
89	15.036	2286	2288	2290	rBV2	290	208	0.00%	0.000%
90	15.103	2295	2299	2301	rBV3	459	460	0.00%	0.000%
91	15.134	2301	2304	2305	rBV2	473	476	0.00%	0.000%
92	15.255	2320	2324	2327	rBV4	374	405	0.00%	0.000%
93	15.286	2327	2329	2330	rBV2	293	236	0.00%	0.000%
94	15.390	2342	2346	2350	rBV3	1012	1656	0.00%	0.000%
95	15.451	2355	2356	2358	rBV	259	222	0.00%	0.000%
96	15.694	2395	2396	2398	rBV2	281	229	0.00%	0.000%
97	16.231	2480	2484	2487	rBV3	299	480	0.00%	0.000%
98	16.280	2489	2492	2494	rBV3	394	478	0.00%	0.000%
99	16.463	2520	2522	2524	rBV3	443	376	0.00%	0.000%
100	16.548	2534	2536	2543	rVB4	512	899	0.00%	0.000%

Sum of corrected areas: 369586318

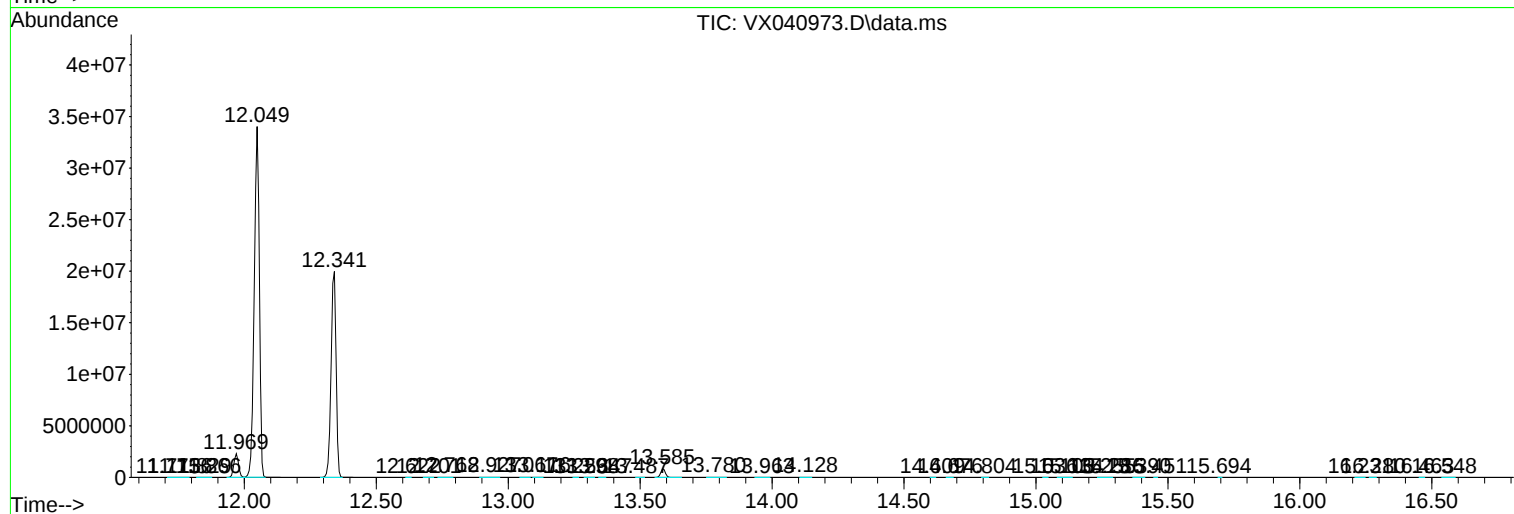
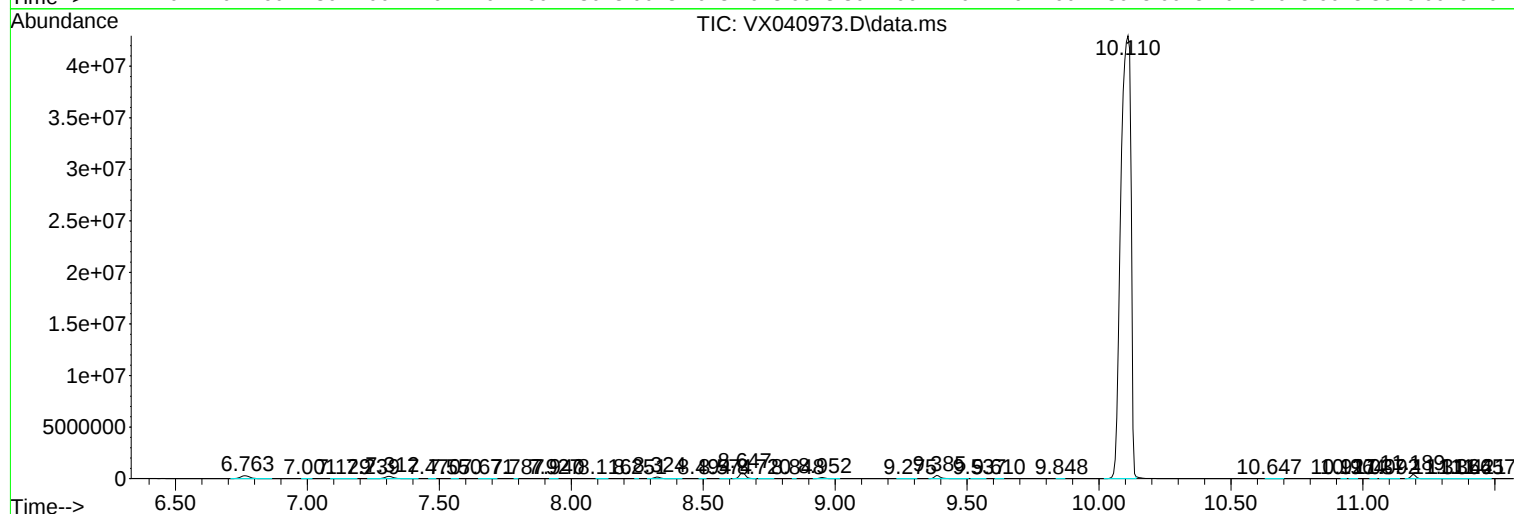
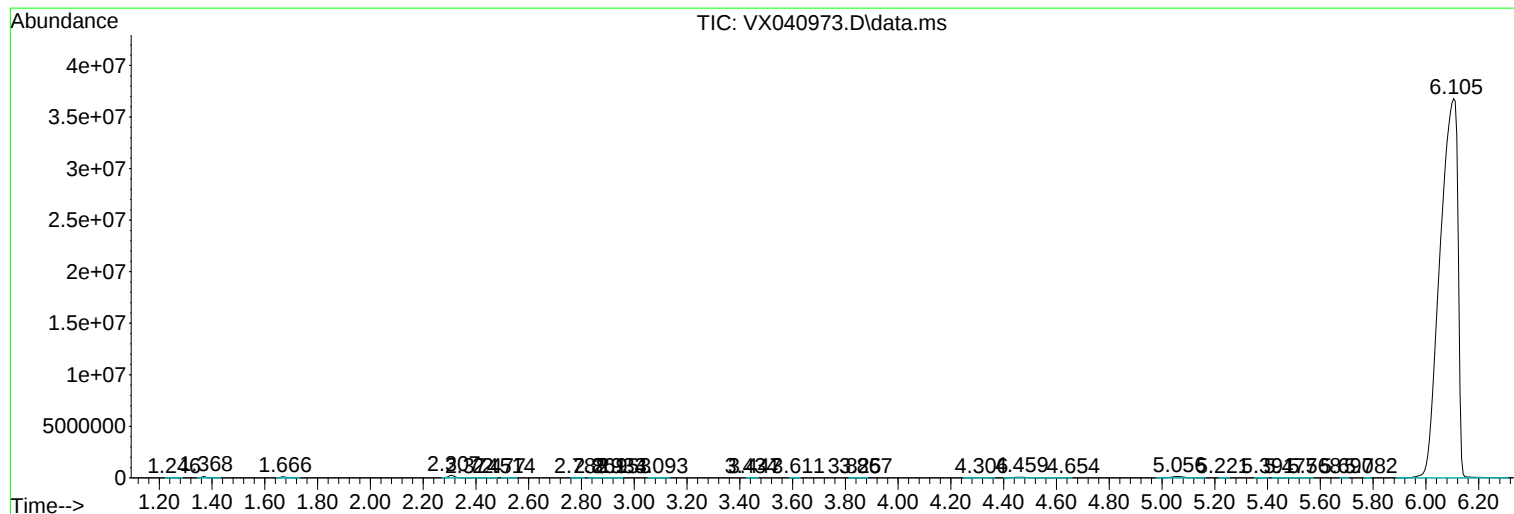
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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MC0R47

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041024WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\WX041124\
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ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_X
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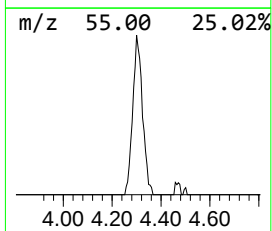
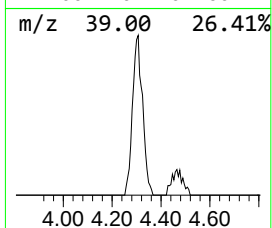
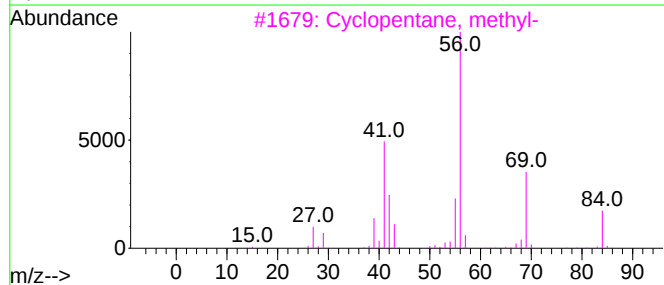
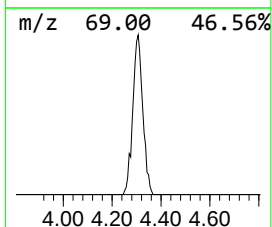
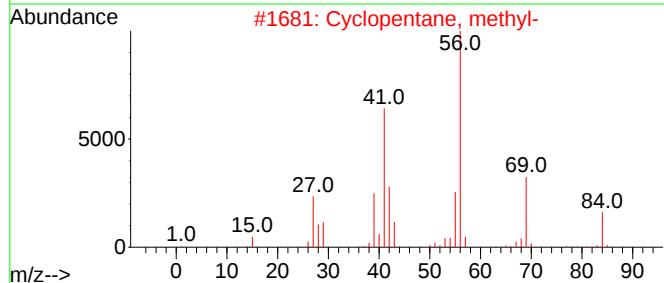
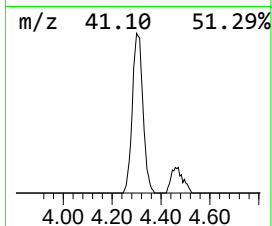
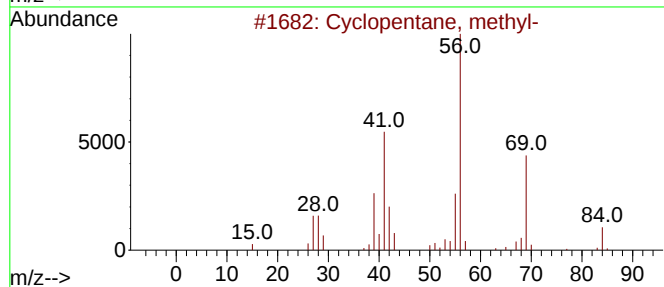
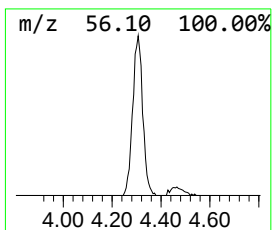
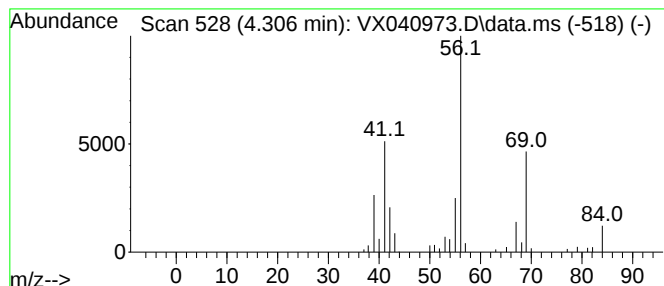
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML041024WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Cyclic4.48 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	4.48 ug/L	59979	1,4-Difluorobenzene	6.763

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			Cyclopentane, methyl-	84	C6H12	000096-37-7	80
4			Cyclopentane, methyl-	84	C6H12	000096-37-7	72
5			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: C...	4.306	4.5	ug/L	59979	1	6.763	670059	50.0