

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122123\
 Data File : VX039427.D
 Acq On : 21 Dec 2023 14:18
 Operator : JC/MD
 Sample : 05807-05
 Misc : 3.19g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AX7

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\SFAMXML120523WMA.M
 Title : VOC Analysis

Signal : TIC: VX039427.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	61	rVB	80054	134193	11.62%	1.417%
2	1.648	89	92	101	rVB	25843	35609	3.08%	0.376%
3	2.288	191	197	210	rVB	227574	358608	31.05%	3.785%
4	2.398	210	215	221	rBV4	2130	4402	0.38%	0.046%
5	2.715	261	267	275	rBV	4601	9315	0.81%	0.098%
6	2.782	275	278	279	rVV3	1522	1744	0.15%	0.018%
7	2.849	282	289	299	rVV	90556	182917	15.84%	1.931%
8	2.941	299	304	318	rVB2	6339	16188	1.40%	0.171%
9	3.069	323	325	327	rBV3	381	416	0.04%	0.004%
10	3.105	330	331	332	rBV	416	228	0.02%	0.002%
11	3.123	332	334	338	rVV3	567	485	0.04%	0.005%
12	3.178	342	343	346	rBV2	173	216	0.02%	0.002%
13	3.251	352	355	359	rBV2	212	263	0.02%	0.003%
14	3.300	359	363	364	rBV4	181	293	0.03%	0.003%
15	3.660	420	422	425	rVB2	339	403	0.03%	0.004%
16	3.879	456	458	460	rBV2	255	224	0.02%	0.002%
17	3.928	463	466	469	rBV2	316	445	0.04%	0.005%
18	4.087	490	492	494	rBV	282	222	0.02%	0.002%
19	4.190	507	509	511	rBV2	239	218	0.02%	0.002%
20	4.337	531	533	536	rVB	222	236	0.02%	0.002%
21	4.477	546	556	590	rBV	72202	319687	27.68%	3.375%
22	4.885	622	623	628	rVB3	200	236	0.02%	0.002%
23	5.056	639	651	670	rBV	138942	461212	39.93%	4.868%
24	5.251	681	683	684	rBV2	334	246	0.02%	0.003%
25	5.373	700	703	705	rBV	404	468	0.04%	0.005%
26	5.544	728	731	732	rBV2	546	428	0.04%	0.005%
27	5.964	788	800	818	rBV2	392686	1154981	100.00%	12.192%
28	6.251	844	847	851	rBV2	221	344	0.03%	0.004%
29	6.281	851	852	856	rVV	422	261	0.02%	0.003%
30	6.531	890	893	896	rBV2	292	419	0.04%	0.004%
31	6.757	921	930	950	rVV	298004	745419	64.54%	7.868%
32	7.031	974	975	977	rVB2	397	247	0.02%	0.003%
33	7.111	983	988	996	rVB4	2147	4591	0.40%	0.048%
34	7.220	1002	1006	1009	rBV2	345	625	0.05%	0.007%
35	7.306	1011	1020	1035	rBV	238116	535582	46.37%	5.653%
36	7.434	1039	1041	1045	rVB4	652	544	0.05%	0.006%

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 Title : VOC Analysis

37	7.470	1045	1047	1050	rBV3	482	764	0.07%	0.008%
38	7.824	1102	1105	1108	rBV	192	238	0.02%	0.003%
39	7.940	1121	1124	1125	rBV2	314	354	0.03%	0.004%
40	8.135	1153	1156	1158	rBV	206	273	0.02%	0.003%
41	8.263	1172	1177	1181	rBV3	719	1190	0.10%	0.013%
42	8.324	1181	1187	1204	rVV	150275	260929	22.59%	2.754%
43	8.507	1215	1217	1223	rVB2	577	880	0.08%	0.009%
44	8.580	1228	1229	1230	rBV	304	206	0.02%	0.002%
45	8.647	1234	1240	1251	rBV	554643	886234	76.73%	9.355%
46	8.952	1285	1290	1306	rVV	106504	172312	14.92%	1.819%
47	9.275	1340	1343	1348	rVB4	1219	1618	0.14%	0.017%
48	9.397	1356	1363	1384	rBV	409307	728769	63.10%	7.693%
49	9.714	1410	1415	1418	rBV4	1113	1606	0.14%	0.017%
50	9.897	1444	1445	1449	rVB2	261	234	0.02%	0.002%
51	9.994	1459	1461	1463	rBV2	210	208	0.02%	0.002%
52	10.055	1465	1471	1474	rBV	648482	1043448	90.34%	11.014%
53	10.201	1492	1495	1501	rVB5	1038	1759	0.15%	0.019%
54	10.311	1508	1513	1518	rBV4	954	1480	0.13%	0.016%
55	10.445	1532	1535	1539	rBV2	226	367	0.03%	0.004%
56	10.488	1539	1542	1543	rBV	231	231	0.02%	0.002%
57	10.592	1556	1559	1562	rVV2	233	292	0.03%	0.003%
58	10.646	1566	1568	1576	rVV4	1200	2220	0.19%	0.023%
59	10.744	1580	1584	1587	rBV2	205	348	0.03%	0.004%
60	10.939	1613	1616	1617	rBV2	321	332	0.03%	0.004%
61	11.098	1640	1642	1644	rVB2	364	282	0.02%	0.003%
62	11.140	1647	1649	1652	rVV2	278	213	0.02%	0.002%
63	11.195	1652	1658	1671	rBV	451750	581472	50.34%	6.138%
64	11.317	1673	1678	1683	rVB2	3065	4651	0.40%	0.049%
65	11.457	1695	1701	1702	rBV3	1112	1233	0.11%	0.013%
66	11.567	1718	1719	1722	rBV	297	224	0.02%	0.002%
67	11.756	1747	1750	1753	rBV2	1020	1508	0.13%	0.016%
68	11.829	1760	1762	1765	rVB2	243	263	0.02%	0.003%
69	11.884	1768	1771	1772	rBV2	298	242	0.02%	0.003%
70	11.945	1777	1781	1782	rBV	233	300	0.03%	0.003%
71	11.976	1782	1786	1788	rVV2	2161	2442	0.21%	0.026%
72	12.024	1788	1794	1806	rVV	725146	940002	81.39%	9.922%
73	12.134	1810	1812	1814	rVB	591	410	0.04%	0.004%
74	12.317	1837	1842	1855	rBV	600235	818548	70.87%	8.640%
75	12.762	1908	1915	1921	rVB2	9654	13542	1.17%	0.143%
76	12.817	1921	1924	1925	rVB	416	230	0.02%	0.002%

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 Title : VOC Analysis

77	12.853	1928	1930	1932	rBV	326	293	0.03%	0.003%
78	13.012	1954	1956	1958	rBV	196	221	0.02%	0.002%
79	13.036	1958	1960	1964	rVB2	287	244	0.02%	0.003%
80	13.122	1970	1974	1980	rVB4	800	1124	0.10%	0.012%
81	13.262	1996	1997	2000	rVB	475	433	0.04%	0.005%
82	13.298	2002	2003	2007	rVB	298	207	0.02%	0.002%
83	13.524	2037	2040	2045	rVB2	285	478	0.04%	0.005%
84	13.591	2047	2051	2057	rBV4	2186	3146	0.27%	0.033%
85	13.780	2079	2082	2088	rVV	686	1114	0.10%	0.012%
86	13.878	2095	2098	2102	rVB2	320	437	0.04%	0.005%
87	13.963	2108	2112	2117	rBV3	1001	1198	0.10%	0.013%
88	14.128	2134	2139	2145	rVB	11934	15702	1.36%	0.166%
89	14.341	2173	2174	2177	rBV	296	261	0.02%	0.003%
90	14.426	2186	2188	2190	rBV2	523	409	0.04%	0.004%
91	14.512	2199	2202	2204	rBV2	333	319	0.03%	0.003%
92	14.670	2227	2228	2230	rBV	288	212	0.02%	0.002%
93	15.103	2298	2299	2301	rVB	379	216	0.02%	0.002%
94	15.249	2322	2323	2326	rVB	550	238	0.02%	0.003%
95	15.390	2343	2346	2351	rVB4	1371	2200	0.19%	0.023%
96	15.444	2353	2355	2356	rBV	398	318	0.03%	0.003%
97	15.957	2437	2439	2440	rBV	249	249	0.02%	0.003%
98	16.048	2453	2454	2456	rBV2	290	229	0.02%	0.002%
99	16.109	2462	2464	2466	rVB2	314	232	0.02%	0.002%
100	16.145	2469	2470	2473	rBV	327	236	0.02%	0.002%

Sum of corrected areas: 9473485

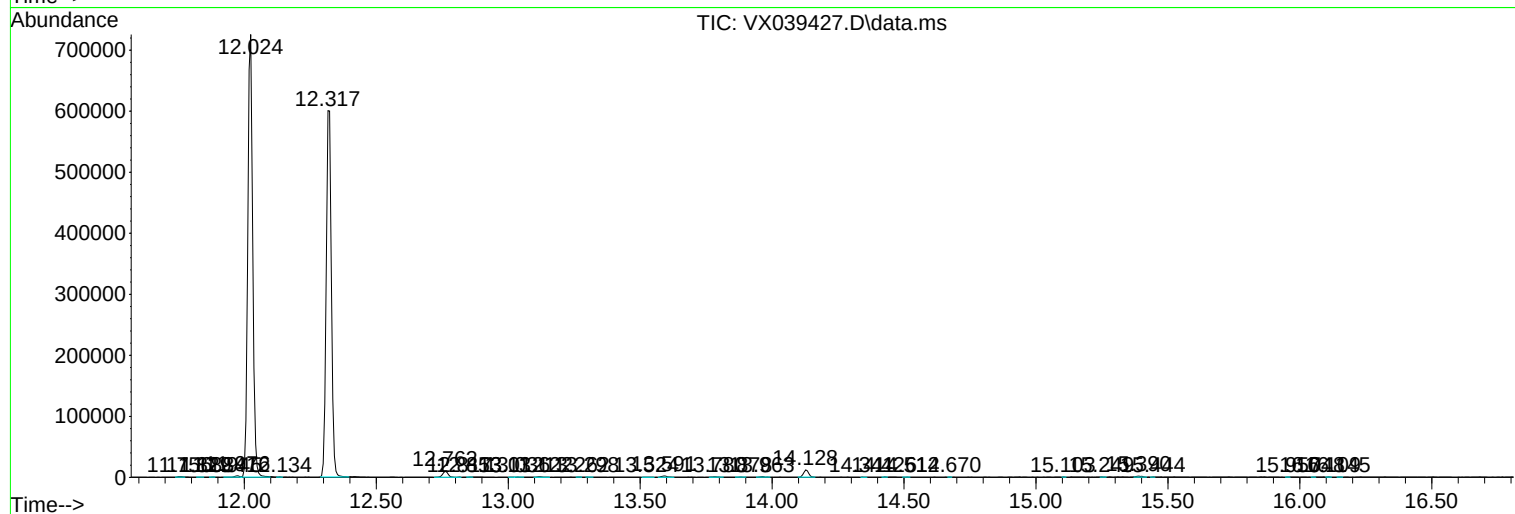
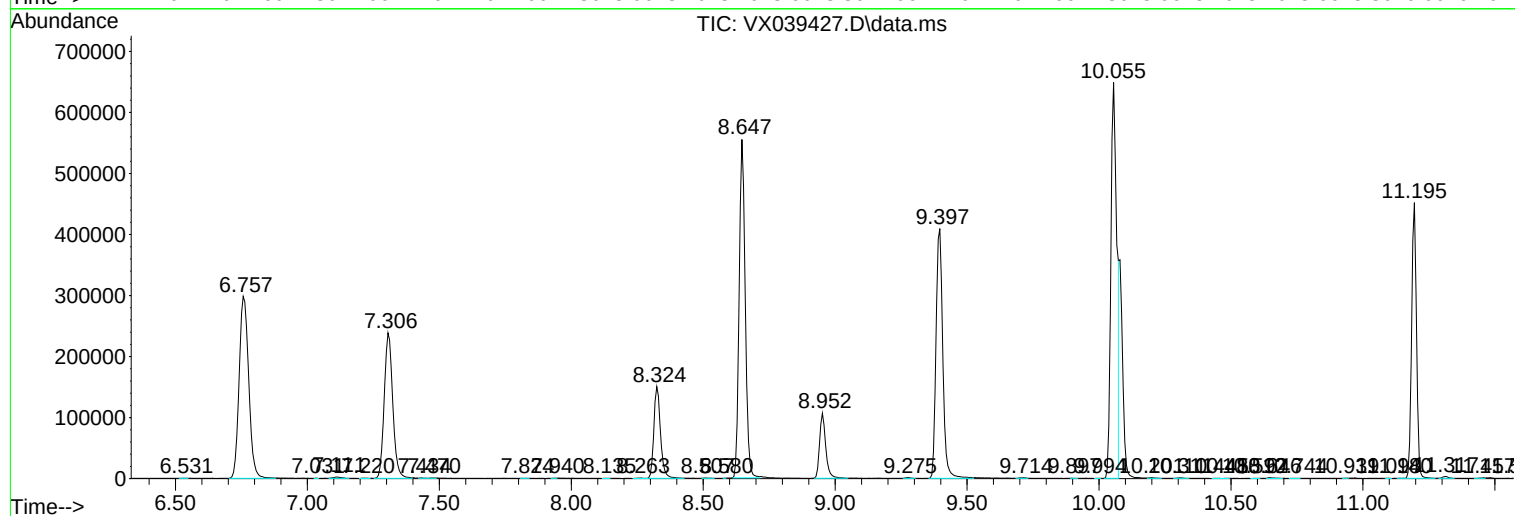
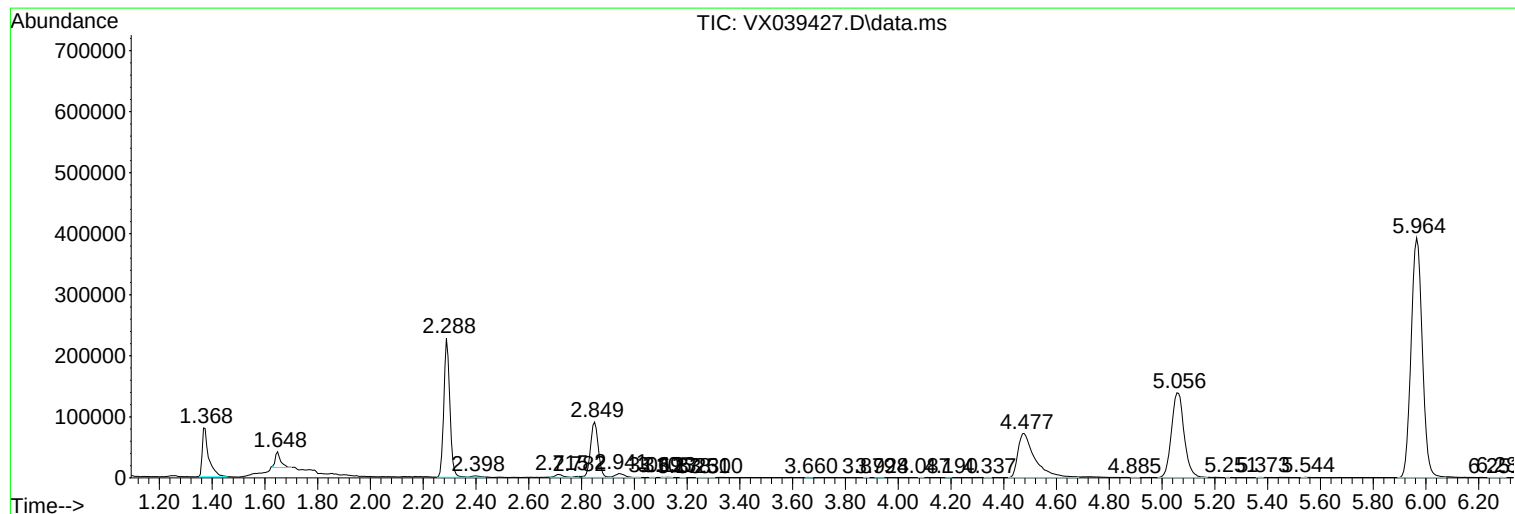
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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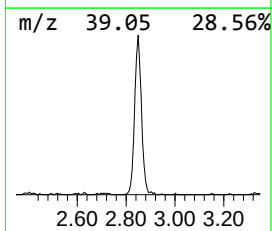
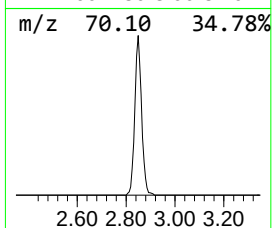
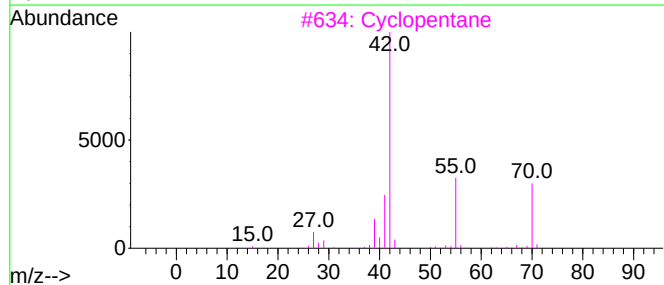
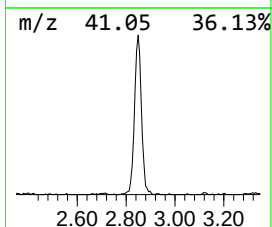
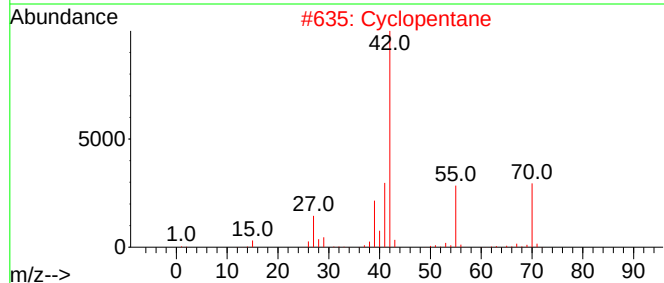
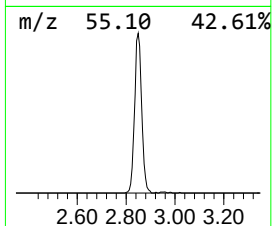
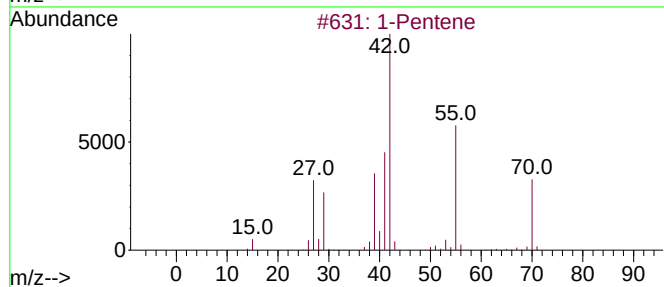
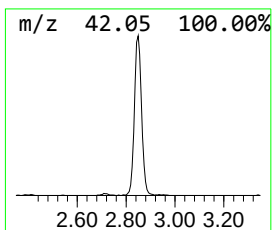
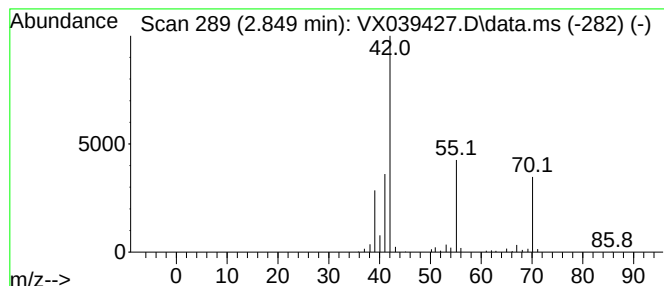
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.849	12.27 ug/L	182917	1,4-Difluorobenzene	6.763	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	91
2	Cyclopentane	70	C5H10	000287-92-3	90
3	Cyclopentane	70	C5H10	000287-92-3	78
4	Cyclobutane, methyl-	70	C5H10	000598-61-8	78
5	Cyclopropane, ethyl-	70	C5H10	001191-96-4	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	2.849	12.3	ug/L	182917	1	6.763	745419	50.0