

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011722\
 Data File : VV024381.D
 Acq On : 17 Jan 2022 17:55
 Operator : SY/MD
 Sample : N1115-12ME 10X
 Misc : 6.05g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BGLS2ME

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_V\Method\SFAMVLM123121WMA.M
 Title : VOC Analysis

Signal : TIC: VV024381.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.217	50	55	61	rBV	27490	24415	1.14%	0.187%
2	1.307	76	83	100	rVB	276510	283493	13.28%	2.177%
3	1.568	157	164	176	rVB	213962	232205	10.88%	1.783%
4	2.108	322	332	362	rVB	480963	713806	33.45%	5.482%
5	2.237	370	372	377	rVB	692	347	0.02%	0.003%
6	2.394	418	421	424	rBV2	343	258	0.01%	0.002%
7	2.536	463	465	467	rVB3	473	145	0.01%	0.001%
8	2.552	468	470	476	rBV2	293	201	0.01%	0.002%
9	2.610	485	488	490	rBV3	615	406	0.02%	0.003%
10	2.674	506	508	515	rVB4	468	266	0.01%	0.002%
11	2.735	524	527	530	rVB2	257	145	0.01%	0.001%
12	2.764	533	536	540	rVB2	785	546	0.03%	0.004%
13	2.783	540	542	546	rBV2	406	207	0.01%	0.002%
14	2.886	572	574	580	rVB3	301	293	0.01%	0.002%
15	2.918	581	584	586	rVV2	225	123	0.01%	0.001%
16	2.960	586	597	610	rVV4	5086	11182	0.52%	0.086%
17	3.063	627	629	631	rBV2	265	182	0.01%	0.001%
18	3.182	660	666	667	rBV2	883	672	0.03%	0.005%
19	3.339	710	715	716	rBV	373	259	0.01%	0.002%
20	3.449	744	749	751	rBV	411	331	0.02%	0.003%
21	3.474	755	757	761	rVB2	438	277	0.01%	0.002%
22	3.497	761	764	768	rBV2	322	296	0.01%	0.002%
23	3.539	775	777	780	rVB2	395	165	0.01%	0.001%
24	3.584	785	791	792	rBV2	359	375	0.02%	0.003%
25	3.622	800	803	806	rBV2	243	198	0.01%	0.002%
26	3.700	824	827	829	rVB2	218	132	0.01%	0.001%
27	3.712	829	831	834	rBV2	326	180	0.01%	0.001%
28	3.754	842	844	849	rVB	321	226	0.01%	0.002%
29	3.780	849	852	855	rVB2	178	121	0.01%	0.001%
30	3.799	855	858	862	rBV	171	124	0.01%	0.001%
31	3.883	872	884	920	rBV	138846	418261	19.60%	3.212%
32	4.275	1004	1006	1008	rVB3	684	204	0.01%	0.002%
33	4.346	1012	1028	1058	rVV	356850	868849	40.71%	6.672%
34	4.667	1126	1128	1130	rBV	444	266	0.01%	0.002%
35	4.786	1163	1165	1166	rBV	334	129	0.01%	0.001%
36	4.831	1175	1179	1181	rBV2	400	307	0.01%	0.002%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
 Title : VOC Analysis

37	5.047	1227	1246	1278	rBV2	821034	2134008	100.00%	16.388%
38	5.323	1328	1332	1336	rBV3	352	366	0.02%	0.003%
39	5.468	1374	1377	1378	rBV2	202	102	0.00%	0.001%
40	5.510	1387	1390	1391	rBV	480	262	0.01%	0.002%
41	5.561	1404	1406	1407	rBV	279	118	0.01%	0.001%
42	5.619	1412	1424	1444	rBV	106279	220147	10.32%	1.691%
43	5.764	1467	1469	1472	rBV3	512	273	0.01%	0.002%
44	5.844	1491	1494	1498	rBV	350	305	0.01%	0.002%
45	5.908	1502	1514	1537	rVV4	41358	99047	4.64%	0.761%
46	6.069	1546	1564	1593	rBV	477040	961936	45.08%	7.387%
47	6.310	1632	1639	1647	rBV9	2989	5344	0.25%	0.041%
48	6.465	1682	1687	1692	rBV4	436	346	0.02%	0.003%
49	6.490	1692	1695	1697	rVB2	394	178	0.01%	0.001%
50	6.519	1697	1704	1706	rBV4	747	984	0.05%	0.008%
51	6.719	1764	1766	1767	rVB	288	97	0.00%	0.001%
52	6.728	1767	1769	1770	rBV	374	143	0.01%	0.001%
53	6.757	1776	1778	1779	rBV	501	190	0.01%	0.001%
54	6.815	1794	1796	1797	rVV	369	157	0.01%	0.001%
55	6.873	1813	1814	1817	rBV	229	130	0.01%	0.001%
56	6.928	1828	1831	1833	rBV2	247	148	0.01%	0.001%
57	6.986	1837	1849	1869	rBV	284971	508127	23.81%	3.902%
58	7.188	1905	1912	1915	rBV6	1068	1401	0.07%	0.011%
59	7.314	1938	1951	1968	rBV	1032117	1784940	83.64%	13.708%
60	7.580	2031	2034	2035	rBV3	539	255	0.01%	0.002%
61	7.619	2036	2046	2068	rVV	200149	340137	15.94%	2.612%
62	7.857	2118	2120	2126	rVB4	635	533	0.02%	0.004%
63	7.976	2145	2157	2172	rBV	161636	272994	12.79%	2.096%
64	8.085	2181	2191	2235	rBV	509112	956916	44.84%	7.349%
65	8.423	2292	2296	2298	rBV3	1362	1202	0.06%	0.009%
66	8.503	2319	2321	2322	rBV2	431	211	0.01%	0.002%
67	8.555	2335	2337	2339	rBV	316	130	0.01%	0.001%
68	8.587	2346	2347	2349	rBV2	333	131	0.01%	0.001%
69	8.648	2363	2366	2368	rBV2	415	270	0.01%	0.002%
70	8.854	2419	2430	2447	rBV	158253	264481	12.39%	2.031%
71	9.014	2478	2480	2481	rBV2	724	316	0.01%	0.002%
72	9.069	2494	2497	2498	rBV2	472	223	0.01%	0.002%
73	9.149	2513	2522	2530	rBV7	2718	4975	0.23%	0.038%
74	9.307	2569	2571	2575	rBV	271	199	0.01%	0.002%
75	9.371	2589	2591	2593	rVB	325	130	0.01%	0.001%
76	9.420	2601	2606	2607	rBV2	271	256	0.01%	0.002%

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Integrator: RTE

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 Title : VOC Analysis

77	9.612	2664	2666	2668	rBV2	280	126	0.01%	0.001%
78	9.648	2676	2677	2680	rBV	288	123	0.01%	0.001%
79	9.680	2680	2687	2690	rBV4	768	842	0.04%	0.006%
80	9.709	2693	2696	2698	rBV	808	471	0.02%	0.004%
81	9.928	2761	2764	2765	rBV	541	290	0.01%	0.002%
82	9.989	2780	2783	2784	rBV2	189	101	0.00%	0.001%
83	10.127	2819	2826	2835	rVB3	6009	9605	0.45%	0.074%
84	10.214	2840	2853	2871	rBV	622840	968824	45.40%	7.440%
85	10.320	2881	2886	2892	rBV6	1210	1954	0.09%	0.015%
86	10.426	2915	2919	2922	rBV3	728	559	0.03%	0.004%
87	10.657	2985	2991	2996	rBV4	1209	1609	0.08%	0.012%
88	10.709	3005	3007	3010	rVB	380	159	0.01%	0.001%
89	10.725	3010	3012	3013	rBV	344	98	0.00%	0.001%
90	10.751	3017	3020	3021	rBV	563	321	0.02%	0.002%
91	10.767	3022	3025	3026	rBV2	859	502	0.02%	0.004%
92	11.030	3098	3107	3114	rBV5	2761	4369	0.20%	0.034%
93	11.249	3165	3175	3194	rBV	164882	268232	12.57%	2.060%
94	11.622	3280	3291	3313	rBV	1041115	1636707	76.70%	12.569%
95	12.246	3482	3485	3488	rBV4	989	784	0.04%	0.006%
96	12.728	3633	3635	3638	rBV	299	214	0.01%	0.002%
97	12.956	3703	3706	3707	rBV2	595	281	0.01%	0.002%
98	13.310	3813	3816	3817	rBV	547	284	0.01%	0.002%
99	13.561	3892	3894	3897	rVB2	1067	511	0.02%	0.004%
100	13.747	3946	3952	3959	rBV6	2128	2909	0.14%	0.022%

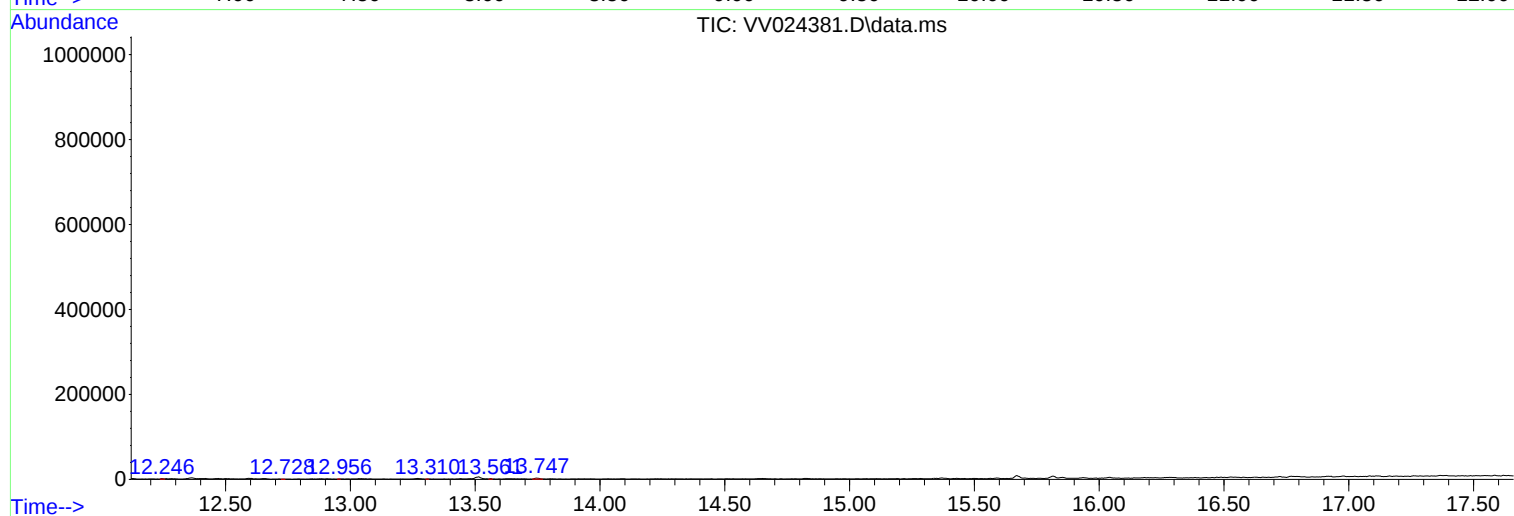
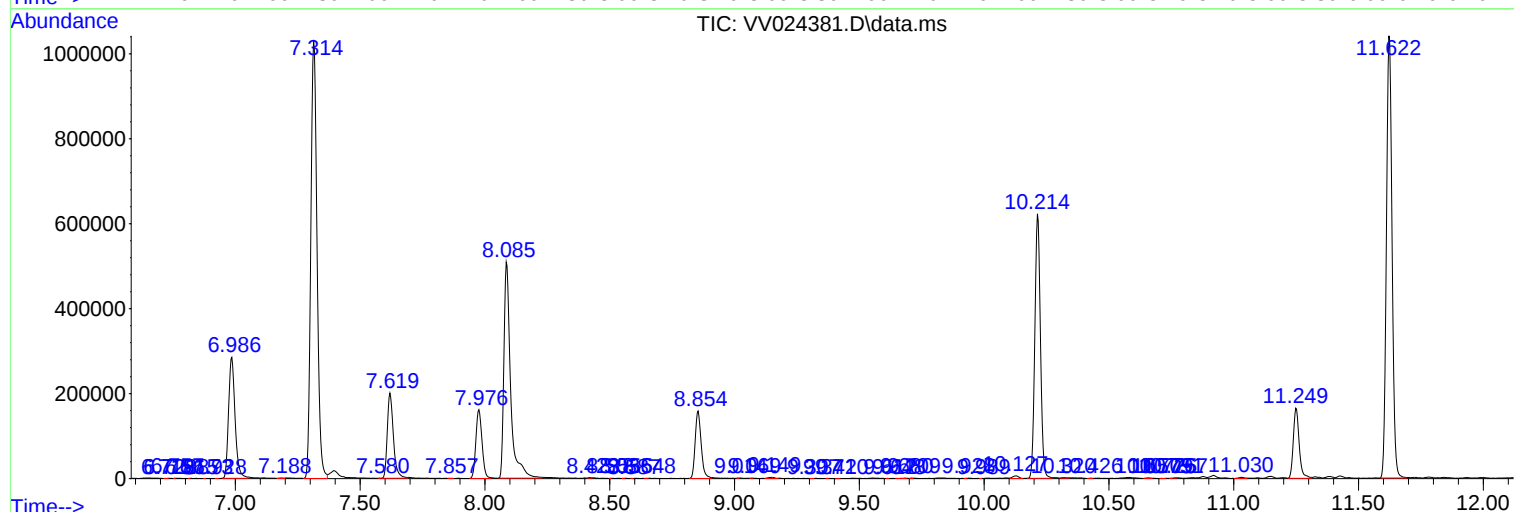
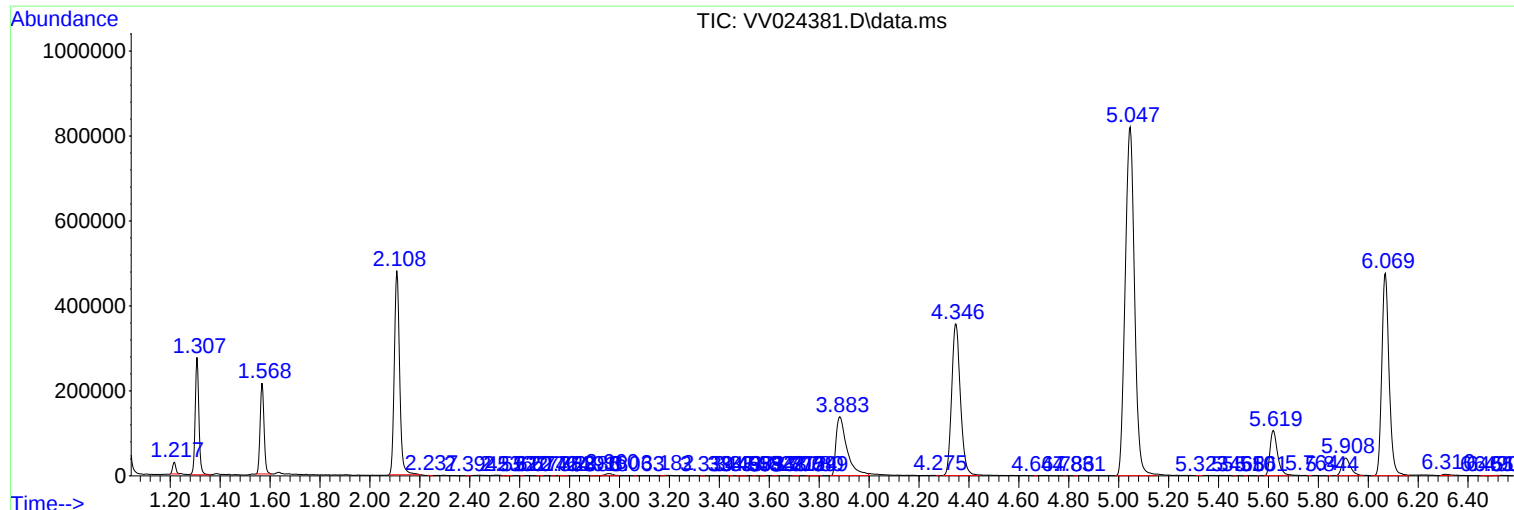
Sum of corrected areas: 13021575

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Instrument :
MSVOA_V
ClientSampleId :
BGLS2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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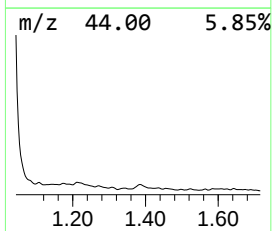
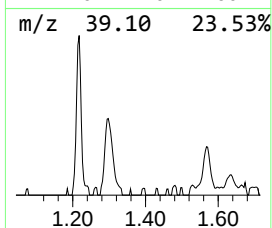
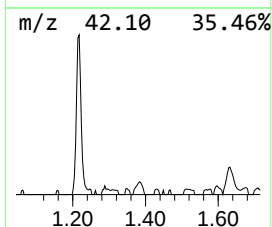
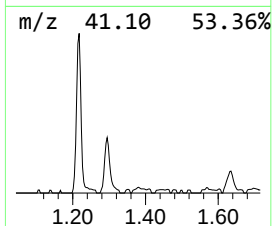
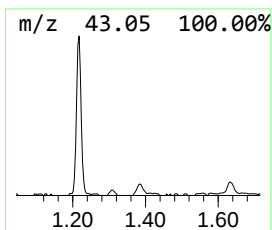
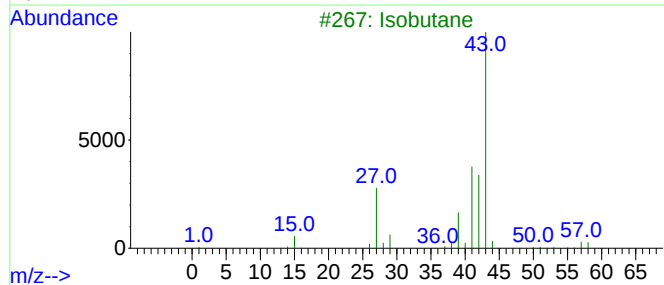
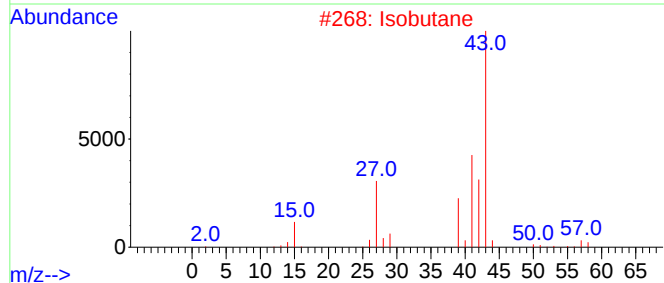
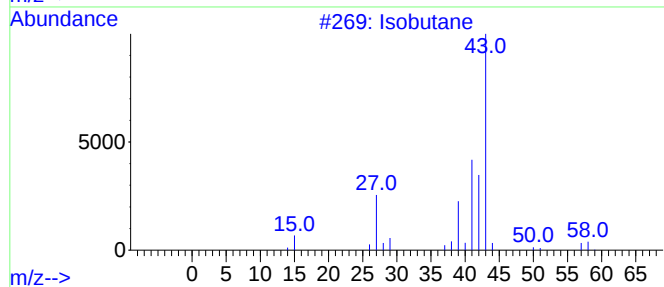
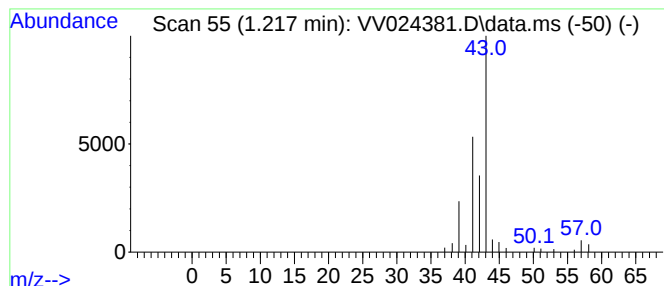
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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.
1.217	5.55 ug/L	24415	1,4-Difluorobenzene	5.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isobutane	58	C4H10	000075-28-5	64
2			Isobutane	58	C4H10	000075-28-5	64
3			Isobutane	58	C4H10	000075-28-5	64
4			Isobutane	58	C4H10	000075-28-5	64
5			Isobutane	58	C4H10	000075-28-5	45



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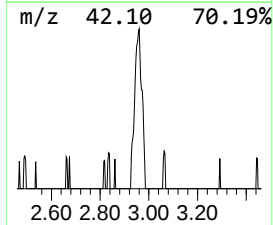
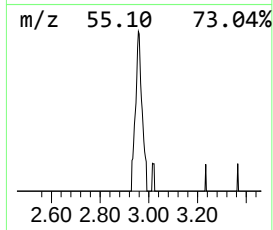
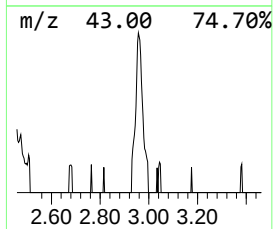
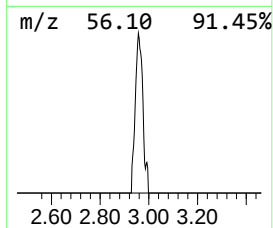
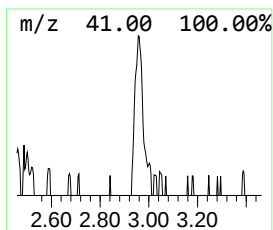
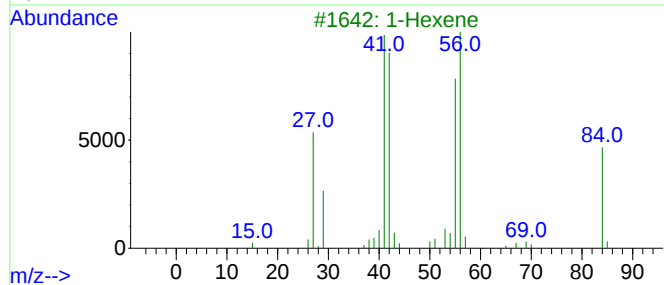
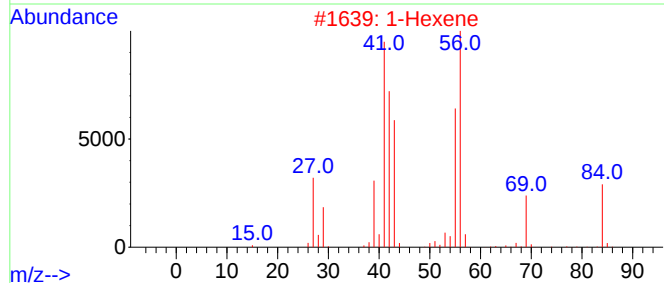
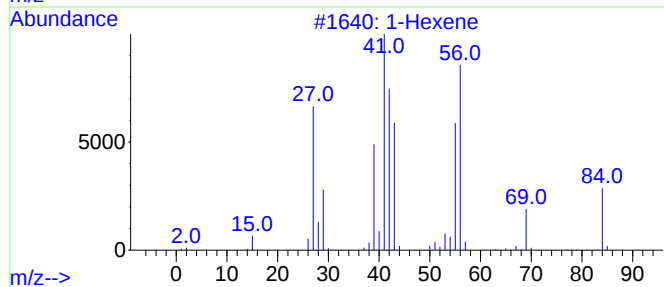
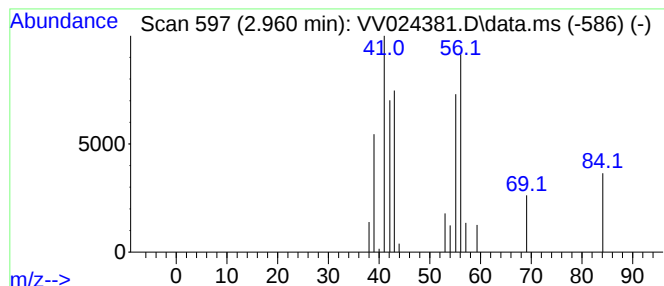
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Quant Title : VOC Analysis

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.
2.960	2.54 ug/L	11182	1,4-Difluorobenzene	5.619

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexene		84	C6H12	000592-41-6	90
2	1-Hexene		84	C6H12	000592-41-6	58
3	1-Hexene		84	C6H12	000592-41-6	50
4	1-Hexanol		102	C6H14O	000111-27-3	50
5	3-Hexene, (E)-		84	C6H12	013269-52-8	43



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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...	1.217	5.5	ug/L	24415	1	5.619	220147	50.0
(DEL) Alkane: S...	2.960	2.5	ug/L	11182	1	5.619	220147	50.0