

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU061120\  
 Data File : VU038795.D  
 Acq On : 10 Jun 2020 22:58  
 Operator : SY/MD  
 Sample : L2915-04 100X  
 Misc : 5.0mL/MSVOA U/WATER  
 ALS Vial : 1 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampled :  
 F9E08

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

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM060820WMA.M  
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.372	5	10	17	rBV2	8847	8287	0.04%	0.021%
2	1.501	44	50	57	rBV2	25448	27072	0.14%	0.068%
3	1.613	74	85	96	rBV3	373144	461171	2.41%	1.162%
4	1.674	98	104	115	rVB	38093	43039	0.23%	0.108%
5	1.748	121	127	136	rVB	34935	40207	0.21%	0.101%
6	1.928	174	183	197	rVB	213515	281426	1.47%	0.709%
7	2.012	201	209	220	rVB2	57070	76671	0.40%	0.193%
8	2.173	251	259	267	rBV	34549	48195	0.25%	0.121%
9	2.224	267	275	292	rVB2	59013	91556	0.48%	0.231%
10	2.340	302	311	327	rVB	34329	52911	0.28%	0.133%
11	2.398	327	329	332	rBV3	1130	996	0.01%	0.003%
12	2.436	333	341	349	rVV2	22263	32102	0.17%	0.081%
13	2.491	349	358	374	rVB	29316	48680	0.25%	0.123%
14	2.591	376	389	410	rBV	466273	787439	4.12%	1.983%
15	2.999	505	516	518	rBV6	2213	3709	0.02%	0.009%
16	3.044	520	530	545	rVB2	28962	56447	0.30%	0.142%
17	3.170	558	569	579	rBV3	31783	63879	0.33%	0.161%
18	3.292	605	607	613	rVB3	854	705	0.00%	0.002%
19	3.353	620	626	629	rBV4	881	971	0.01%	0.002%
20	3.395	632	639	651	rVB9	3403	6427	0.03%	0.016%
21	3.623	699	710	712	rBV4	3121	4845	0.03%	0.012%
22	3.739	734	746	748	rBV6	2054	3508	0.02%	0.009%
23	3.870	774	787	789	rBV5	968	1501	0.01%	0.004%
24	3.887	789	792	800	rVB3	849	810	0.00%	0.002%
25	3.938	803	808	809	rBV	1814	1016	0.01%	0.003%
26	4.009	824	830	832	rBV3	1682	1605	0.01%	0.004%
27	4.215	884	894	908	rVB7	3674	8569	0.04%	0.022%
28	4.292	911	918	920	rBV5	710	845	0.00%	0.002%
29	4.568	985	1004	1019	rBV4	25417	61515	0.32%	0.155%
30	4.665	1019	1034	1066	rBV	246254	640595	3.35%	1.614%
31	4.845	1087	1090	1093	rBV4	637	518	0.00%	0.001%
32	5.102	1152	1170	1192	rBV	392782	850953	4.45%	2.143%
33	5.330	1230	1241	1250	rVB4	1933	3166	0.02%	0.008%
34	5.423	1255	1270	1286	rBV3	41791	93936	0.49%	0.237%

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## Integration Parameters: LSCINT.P

Integrator: RTE  
 Smoothing : OFF  
 Sampling : 1  
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Filtering: 5  
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If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
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Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM060820WMA.M  
 Title : VOC Analysis

35	5.761	1351	1375	1378	rBV3	817939	1887077	9.87%	4.753%
36	5.809	1379	1390	1421	rVB	9462014	19114762	100.00%	48.148%
37	6.279	1522	1536	1569	rVB	684985	1300973	6.81%	3.277%
38	6.423	1578	1581	1586	rVB3	760	603	0.00%	0.002%
39	6.562	1613	1624	1638	rBV4	12767	34556	0.18%	0.087%
40	6.719	1659	1673	1690	rBV	495549	956581	5.00%	2.410%
41	6.877	1719	1722	1728	rVB4	708	506	0.00%	0.001%
42	6.980	1751	1754	1760	rVV2	530	512	0.00%	0.001%
43	7.195	1813	1821	1822	rBV4	1811	1831	0.01%	0.005%
44	7.211	1822	1826	1834	rVB4	3670	4196	0.02%	0.011%
45	7.272	1841	1845	1850	rBV2	513	504	0.00%	0.001%
46	7.417	1881	1890	1899	rBV3	1737	2080	0.01%	0.005%
47	7.591	1929	1944	1964	rVV	272770	476556	2.49%	1.200%
48	7.719	1974	1984	1994	rVB7	3629	7804	0.04%	0.020%
49	7.774	1994	2001	2011	rBV6	2479	4436	0.02%	0.011%
50	7.812	2011	2013	2021	rVB4	905	909	0.00%	0.002%
51	7.922	2031	2047	2059	rBV	924844	1648213	8.62%	4.152%
52	7.992	2060	2069	2094	rVB	324159	601245	3.15%	1.514%
53	8.121	2102	2109	2121	rVB2	14435	23141	0.12%	0.058%
54	8.201	2121	2134	2148	rBV	193999	322097	1.69%	0.811%
55	8.291	2153	2162	2177	rVB2	10377	19475	0.10%	0.049%
56	8.655	2259	2275	2316	rVV	739242	1348896	7.06%	3.398%
57	8.812	2316	2324	2335	rVV6	6125	11195	0.06%	0.028%
58	8.854	2335	2337	2341	rVV3	620	532	0.00%	0.001%
59	8.935	2356	2362	2368	rVV4	953	1236	0.01%	0.003%
60	8.970	2371	2373	2378	rVB3	690	543	0.00%	0.001%
61	9.433	2503	2517	2551	rBV	937297	1659483	8.68%	4.180%
62	9.587	2552	2565	2587	rVV	748071	1213525	6.35%	3.057%
63	9.709	2589	2603	2624	rVB	169025	299427	1.57%	0.754%
64	9.841	2635	2644	2650	rBV7	10491	17112	0.09%	0.043%
65	9.963	2674	2682	2690	rVB3	6923	9903	0.05%	0.025%
66	10.028	2693	2702	2706	rBV5	7358	11045	0.06%	0.028%
67	10.115	2719	2729	2744	rVB	177183	288615	1.51%	0.727%
68	10.298	2780	2786	2792	rVB5	2627	3742	0.02%	0.009%
69	10.349	2795	2802	2806	rBV4	1903	2515	0.01%	0.006%
70	10.381	2806	2812	2820	rVV5	2811	4172	0.02%	0.011%
71	10.443	2823	2831	2837	rVV5	3784	4939	0.03%	0.012%

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 Title : VOC Analysis

72	10.497	2840	2848	2858	rVV	12166	17865	0.09%	0.045%
73	10.664	2893	2900	2906	rVB7	3095	4801	0.03%	0.012%
74	10.771	2920	2933	2954	rBV	681738	1092835	5.72%	2.753%
75	10.918	2968	2979	2987	rBV2	10481	16690	0.09%	0.042%
76	11.008	2989	3007	3013	rBV3	16190	36307	0.19%	0.091%
77	11.098	3027	3035	3048	rVB6	3867	5811	0.03%	0.015%
78	11.217	3064	3072	3081	rVB4	931	1536	0.01%	0.004%
79	11.301	3090	3098	3110	rBV3	18812	30135	0.16%	0.076%
80	11.417	3123	3134	3141	rBV7	3517	5505	0.03%	0.014%
81	11.478	3142	3153	3164	rVB3	25910	37276	0.20%	0.094%
82	11.526	3166	3168	3171	rBV3	1018	563	0.00%	0.001%
83	11.735	3229	3233	3242	rBV7	877	1092	0.01%	0.003%
84	11.822	3247	3260	3276	rBV	1006127	1576363	8.25%	3.971%
85	11.906	3277	3286	3296	rVB	24006	36398	0.19%	0.092%
86	11.960	3296	3303	3304	rBV4	758	716	0.00%	0.002%
87	12.105	3337	3348	3361	rBV	14046	22543	0.12%	0.057%
88	12.205	3365	3379	3393	rBV	994005	1615180	8.45%	4.069%
89	12.320	3410	3415	3426	rVB5	4254	5585	0.03%	0.014%
90	12.455	3450	3457	3460	rBV2	571	651	0.00%	0.002%
91	12.690	3526	3530	3532	rBV3	1503	1202	0.01%	0.003%
92	12.790	3558	3561	3566	rBV2	749	699	0.00%	0.002%
93	12.986	3619	3622	3632	rVB2	804	946	0.00%	0.002%
94	13.037	3634	3638	3642	rBV5	797	755	0.00%	0.002%
95	13.468	3766	3772	3781	rBV6	3768	5871	0.03%	0.015%
96	13.651	3822	3829	3835	rBV5	2217	3309	0.02%	0.008%
97	14.111	3961	3972	3986	rBV	44374	72212	0.38%	0.182%
98	14.237	4001	4011	4019	rBV	6768	9451	0.05%	0.024%
99	15.452	4385	4389	4399	rVB6	4581	5856	0.03%	0.015%
100	16.188	4616	4618	4621	rBV3	1569	1243	0.01%	0.003%

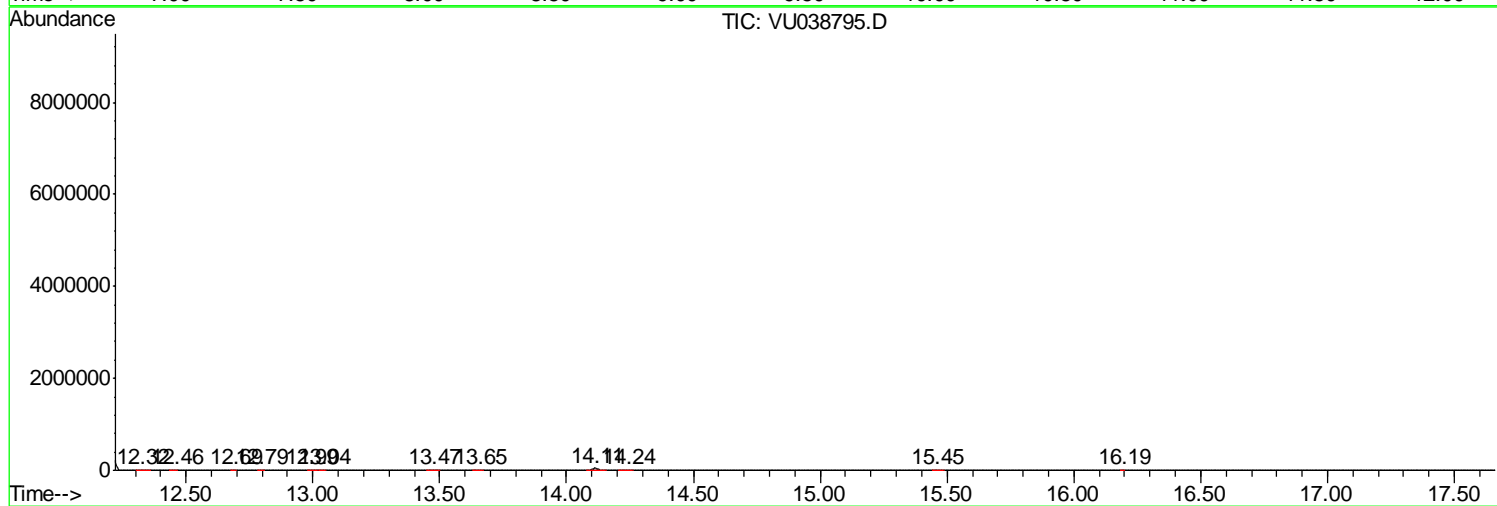
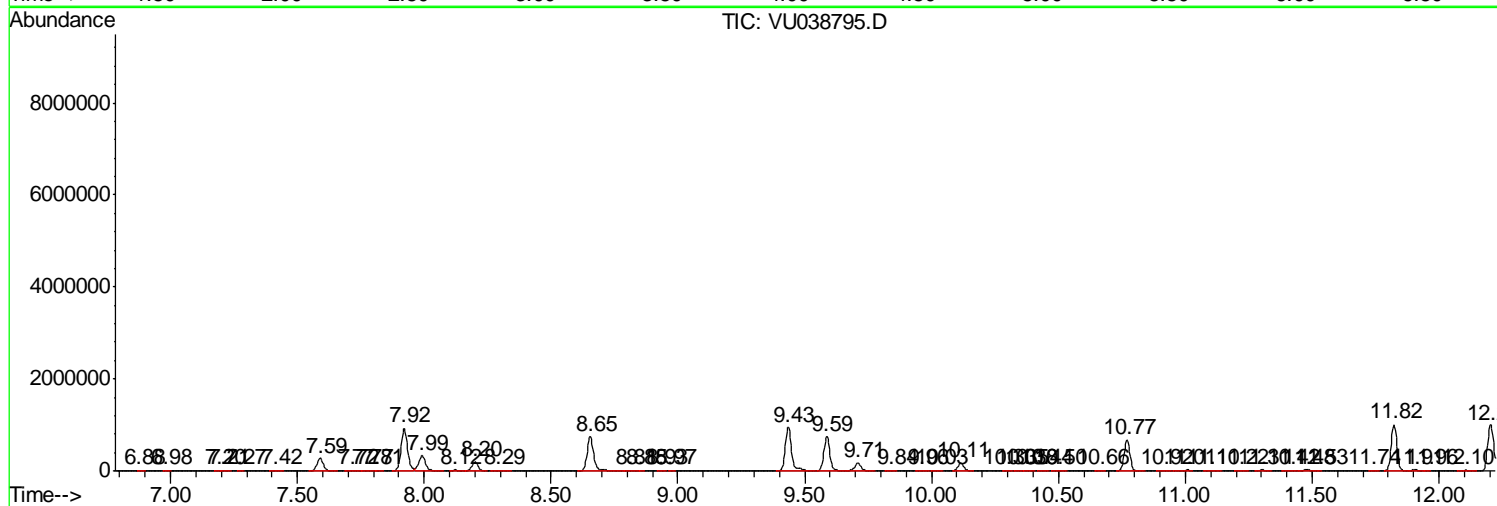
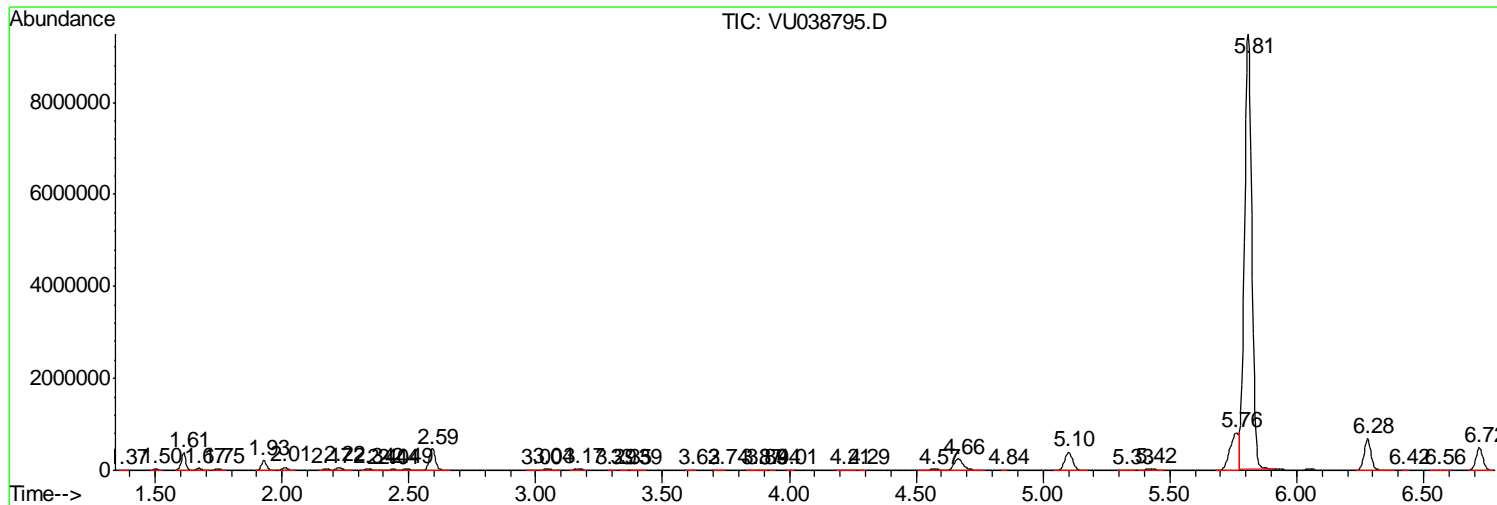
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM060820WMA.M  
 Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P



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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMULM060820WMA.M  
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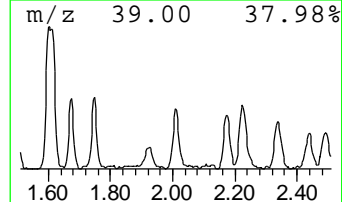
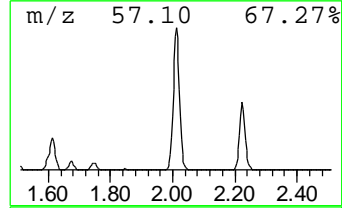
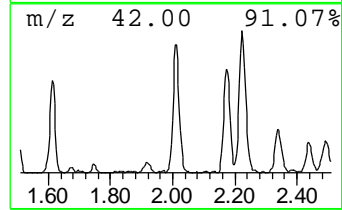
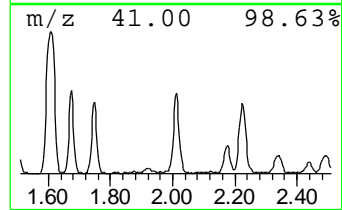
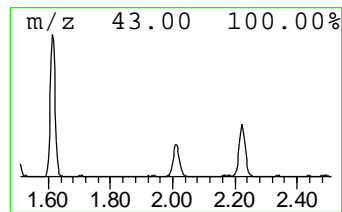
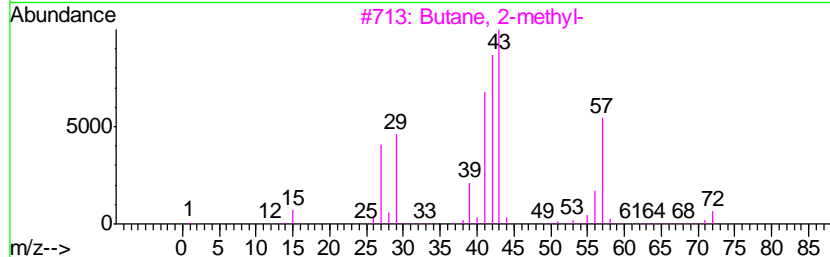
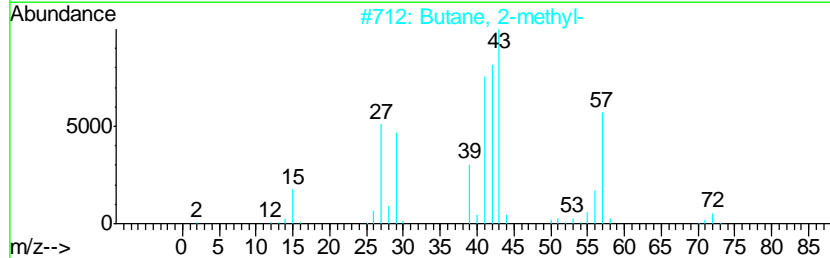
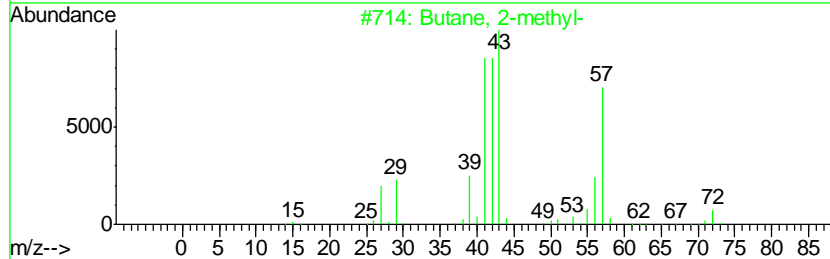
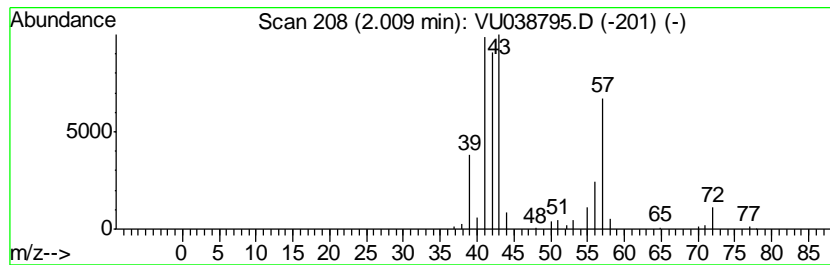
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
 Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.01	2.95 ug/L	76671	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2		Butane, 2-methyl-	72	C5H12	000078-78-4	80
3		Butane, 2-methyl-	72	C5H12	000078-78-4	72
4		3-Buten-1-ol	72	C4H8O	000627-27-0	47
5		Pentane	72	C5H12	000109-66-0	40



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 Quant Title : VOC Analysis

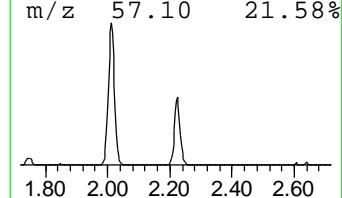
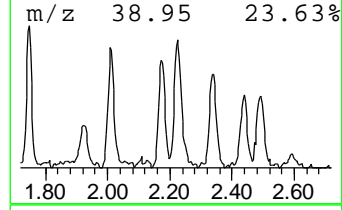
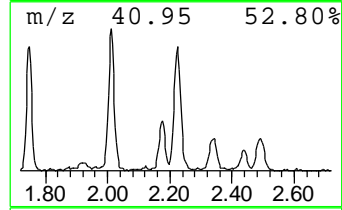
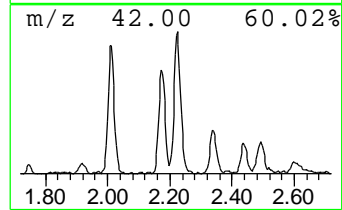
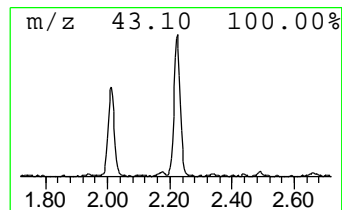
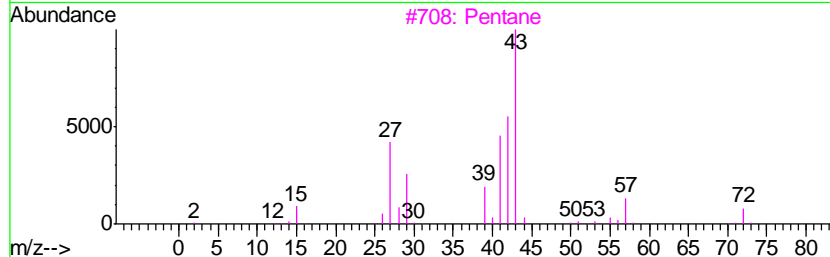
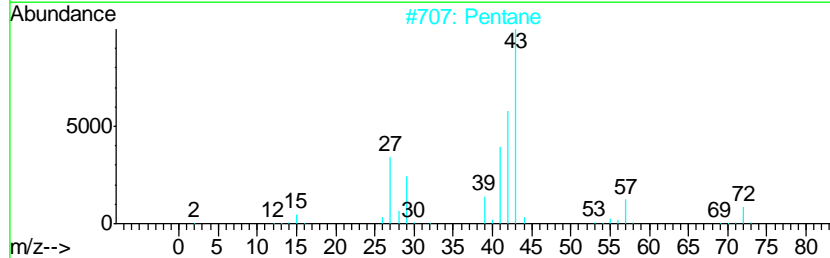
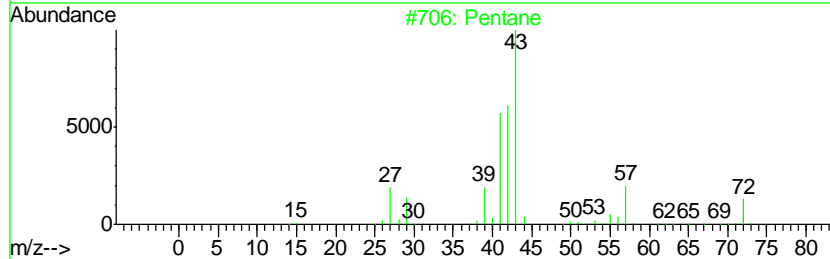
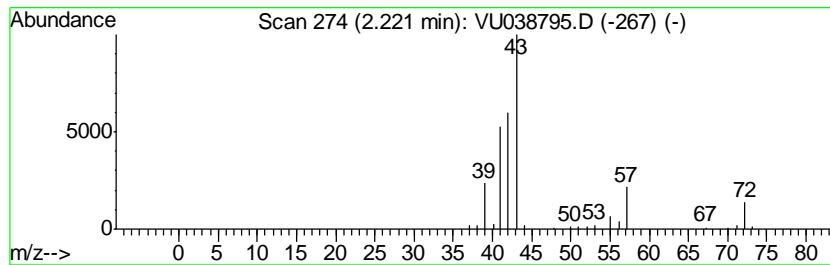
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.22	3.52 ug/L	91556	1,4-Difluorobenzene	6.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane	72	C5H12	000109-66-0	87
2		Pentane	72	C5H12	000109-66-0	80
3		Pentane	72	C5H12	000109-66-0	78
4		Pentane	72	C5H12	000109-66-0	72
5		Oxirane, ethyl-	72	C4H8O	000106-88-7	50



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Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: Str...	2.01	3.0	ug/L	76671	1	6.28	1300970	50.0
(DEL) Alkane: Str...	2.22	3.5	ug/L	91556	1	6.28	1300970	50.0