

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU042919\
 Data File : VU031597.D
 Acq On : 29 Apr 2019 19:24
 Operator : JC/SP
 Sample : K2536-21
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0X09

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\SOMULM042719WMA.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	1.177	22	27	39	rVB2	84412	83733	0.76%	0.230%
2	1.289	59	62	68	rVB2	18864	16254	0.15%	0.045%
3	1.395	87	95	109	rBV	441131	499083	4.53%	1.370%
4	1.678	175	183	196	rBV	367735	458903	4.17%	1.260%
5	1.829	224	230	238	rVV	41663	51886	0.47%	0.142%
6	1.884	239	247	258	rVB	179074	250027	2.27%	0.686%
7	2.270	356	367	379	rBV	721970	1120299	10.17%	3.075%
8	2.836	531	543	553	rBV2	8859	18144	0.16%	0.050%
9	2.900	561	563	568	rVB2	1695	1036	0.01%	0.003%
10	2.974	577	586	587	rBV6	3393	3922	0.04%	0.011%
11	3.080	617	619	623	rBV2	1019	668	0.01%	0.002%
12	3.161	637	644	649	rBV3	1579	2363	0.02%	0.006%
13	3.273	676	679	682	rVB4	984	615	0.01%	0.002%
14	3.292	682	685	687	rBV2	799	564	0.01%	0.002%
15	3.341	695	700	701	rBV3	690	591	0.01%	0.002%
16	3.373	708	710	714	rVV2	814	523	0.00%	0.001%
17	3.434	727	729	734	rVB4	712	539	0.00%	0.001%
18	3.460	734	737	740	rBV3	1626	927	0.01%	0.003%
19	3.479	740	743	745	rBV	981	473	0.00%	0.001%
20	3.492	745	747	751	rBV3	734	648	0.01%	0.002%
21	3.611	781	784	787	rBV2	1166	1025	0.01%	0.003%
22	3.649	792	796	797	rVV3	1237	819	0.01%	0.002%
23	3.672	801	803	808	rVB3	2060	1385	0.01%	0.004%
24	3.701	808	812	815	rBV3	1474	1197	0.01%	0.003%
25	3.791	837	840	843	rBV2	1182	788	0.01%	0.002%
26	3.845	854	857	859	rVB2	1153	698	0.01%	0.002%
27	3.865	859	863	866	rVB3	1960	1714	0.02%	0.005%
28	3.900	870	874	878	rBV4	1168	1194	0.01%	0.003%
29	3.981	894	899	902	rBV5	1204	1432	0.01%	0.004%
30	4.022	908	912	916	rBV2	938	751	0.01%	0.002%
31	4.048	916	920	922	rBV3	1094	846	0.01%	0.002%
32	4.128	942	945	950	rBV5	1082	1135	0.01%	0.003%
33	4.186	950	963	1004	rBV	313843	1147165	10.41%	3.149%
34	4.389	1020	1026	1053	rVB2	32319	89386	0.81%	0.245%

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 Title : VOC Analysis

35	4.643	1089	1105	1132	rBV	539144	1292015	11.73%	3.546%
36	4.807	1153	1156	1158	rBV3	1478	1022	0.01%	0.003%
37	4.871	1172	1176	1177	rBV3	1873	1380	0.01%	0.004%
38	4.977	1206	1209	1218	rBV7	2427	3516	0.03%	0.010%
39	5.132	1247	1257	1264	rBV7	3477	6342	0.06%	0.017%
40	5.202	1276	1279	1287	rVB4	1913	1659	0.02%	0.005%
41	5.334	1296	1320	1360	rBV2	1084062	3358067	30.48%	9.217%
42	5.881	1477	1490	1509	rBV	824538	1672128	15.18%	4.590%
43	6.180	1568	1583	1614	rBV	5576607	11016314	100.00%	30.238%
44	6.324	1618	1628	1662	rVB	761699	1594004	14.47%	4.375%
45	6.765	1763	1765	1769	rBV4	1292	1095	0.01%	0.003%
46	6.852	1790	1792	1797	rVB4	1805	1123	0.01%	0.003%
47	6.897	1803	1806	1811	rVB5	2166	2027	0.02%	0.006%
48	7.045	1849	1852	1853	rVV3	887	546	0.00%	0.001%
49	7.080	1857	1863	1866	rBV6	1340	1452	0.01%	0.004%
50	7.096	1866	1868	1873	rVB5	1759	1475	0.01%	0.004%
51	7.122	1873	1876	1879	rBV3	1318	1164	0.01%	0.003%
52	7.173	1890	1892	1895	rVB3	1286	710	0.01%	0.002%
53	7.225	1896	1908	1931	rBV	370211	698084	6.34%	1.916%
54	7.562	2000	2013	2058	rBV	1264114	2401522	21.80%	6.592%
55	7.849	2090	2102	2121	rBV	244128	455935	4.14%	1.251%
56	8.067	2165	2170	2171	rBV3	2308	1908	0.02%	0.005%
57	8.109	2181	2183	2186	rBV2	623	471	0.00%	0.001%
58	8.128	2186	2189	2191	rBV2	1228	824	0.01%	0.002%
59	8.144	2191	2194	2196	rBV4	1660	1102	0.01%	0.003%
60	8.225	2207	2219	2235	rBV2	425389	745759	6.77%	2.047%
61	8.312	2235	2246	2290	rVB	1001646	2043084	18.55%	5.608%
62	8.710	2363	2370	2374	rBV5	2104	2976	0.03%	0.008%
63	8.810	2397	2401	2408	rBV7	1086	1136	0.01%	0.003%
64	8.871	2418	2420	2425	rBV2	1498	972	0.01%	0.003%
65	9.012	2460	2464	2467	rBV3	818	635	0.01%	0.002%
66	9.086	2473	2487	2525	rBV	1234439	2164197	19.65%	5.940%
67	9.308	2552	2556	2563	rBV8	1685	2015	0.02%	0.006%
68	9.421	2589	2591	2594	rBV3	857	621	0.01%	0.002%
69	9.456	2598	2602	2604	rVV4	1671	1465	0.01%	0.004%
70	9.578	2637	2640	2643	rBV2	1237	793	0.01%	0.002%
71	9.633	2655	2657	2663	rVB4	1662	1345	0.01%	0.004%

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72	9.662	2664	2666	2669	rVB3	1209	634	0.01%	0.002%
73	9.684	2669	2673	2677	rBV5	1491	1162	0.01%	0.003%
74	9.749	2688	2693	2696	rBV4	1398	1342	0.01%	0.004%
75	9.768	2696	2699	2703	rVB3	2565	2176	0.02%	0.006%
76	9.797	2703	2708	2713	rBV6	2014	2583	0.02%	0.007%
77	9.926	2746	2748	2753	rBV2	689	488	0.00%	0.001%
78	10.070	2790	2793	2795	rBV2	943	668	0.01%	0.002%
79	10.135	2810	2813	2814	rBV2	921	578	0.01%	0.002%
80	10.218	2832	2839	2845	rBV9	3876	5964	0.05%	0.016%
81	10.244	2845	2847	2857	rVB6	3179	3950	0.04%	0.011%
82	10.308	2861	2867	2871	rBV6	1503	1612	0.01%	0.004%
83	10.376	2886	2888	2890	rBV3	888	500	0.00%	0.001%
84	10.427	2892	2904	2928	rVV	945261	1534530	13.93%	4.212%
85	10.607	2948	2960	2967	rBV5	7088	10791	0.10%	0.030%
86	10.897	3044	3050	3054	rVB3	1929	2549	0.02%	0.007%
87	11.192	3136	3142	3147	rVB4	2314	2998	0.03%	0.008%
88	11.231	3147	3154	3155	rBV2	1052	1076	0.01%	0.003%
89	11.247	3156	3159	3162	rVB	1735	1252	0.01%	0.003%
90	11.299	3168	3175	3176	rBV5	1419	1500	0.01%	0.004%
91	11.405	3205	3208	3210	rBV2	1554	936	0.01%	0.003%
92	11.479	3220	3231	3258	rBV	981865	1613947	14.65%	4.430%
93	11.749	3305	3315	3333	rBV2	57396	135666	1.23%	0.372%
94	11.855	3337	3348	3377	rVB	1103700	1852971	16.82%	5.086%
95	13.012	3703	3708	3710	rBV3	2302	2007	0.02%	0.006%
96	13.253	3781	3783	3787	rBV2	2294	2071	0.02%	0.006%
97	13.395	3824	3827	3830	rBV4	1885	1362	0.01%	0.004%
98	13.771	3941	3944	3948	rBV3	1938	1834	0.02%	0.005%
99	13.909	3984	3987	3991	rBV3	1975	1585	0.01%	0.004%
100	13.980	4006	4009	4014	rBV5	1860	2041	0.02%	0.006%

Sum of corrected areas: 36432389

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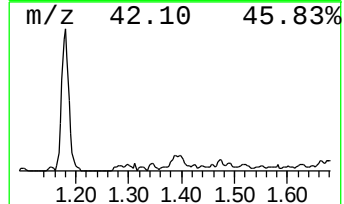
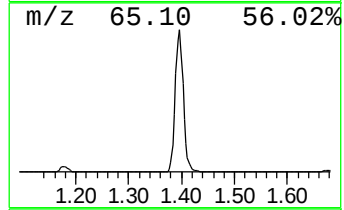
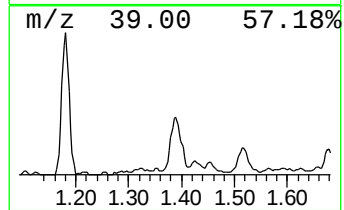
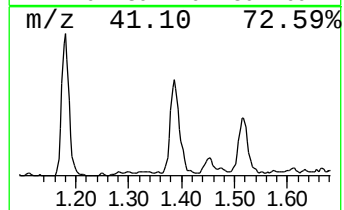
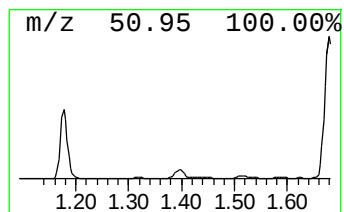
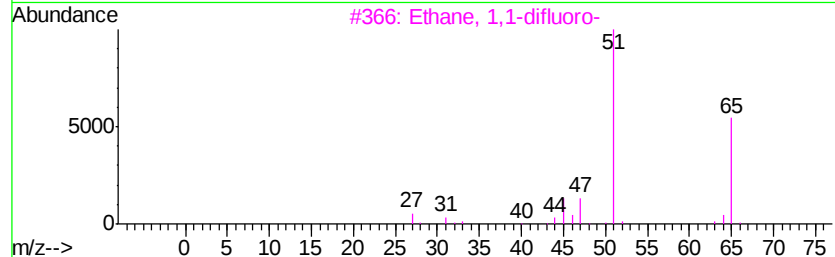
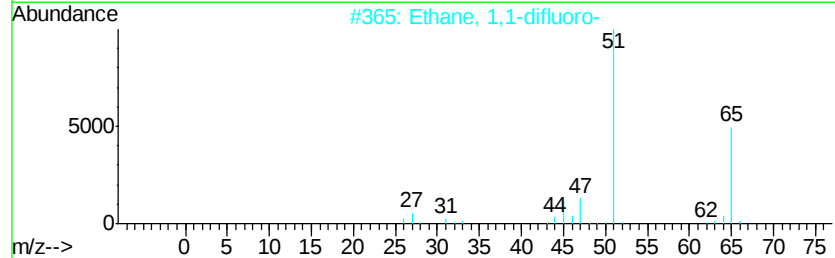
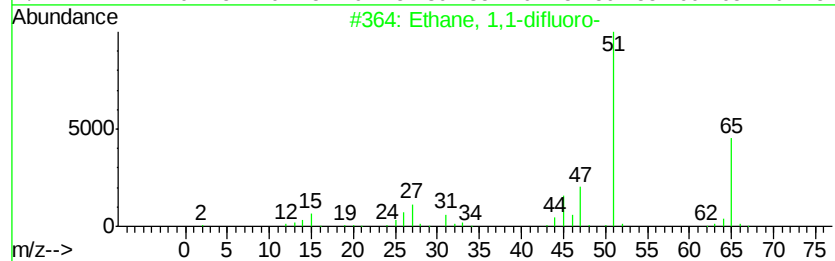
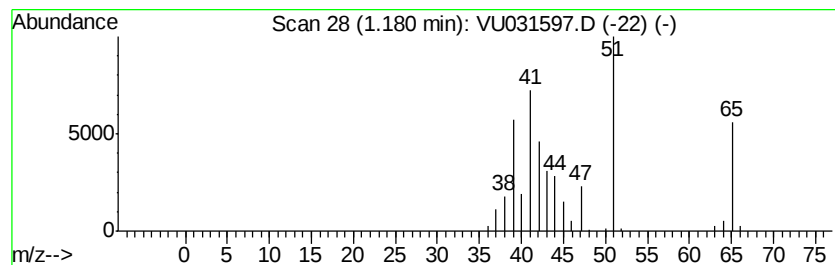
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042719WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Ethane, 1,1-difluoro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.18	2.50 ug/L	83733	1,4-Difluorobenzene	5.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	87
2			Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	80
3			Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	56
4			Propiolonitrile	51	C3HN	001070-71-9	3
5			Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	2



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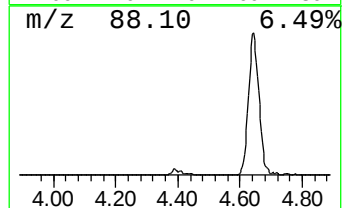
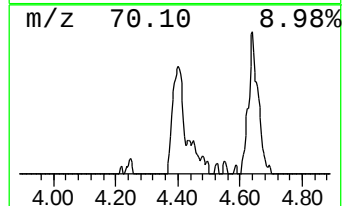
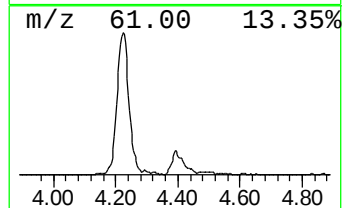
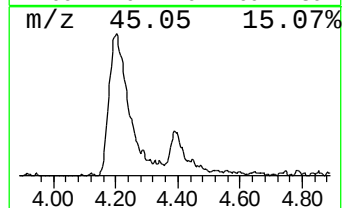
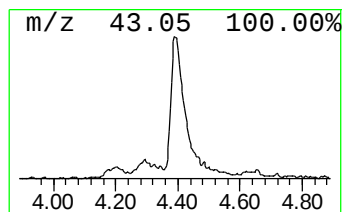
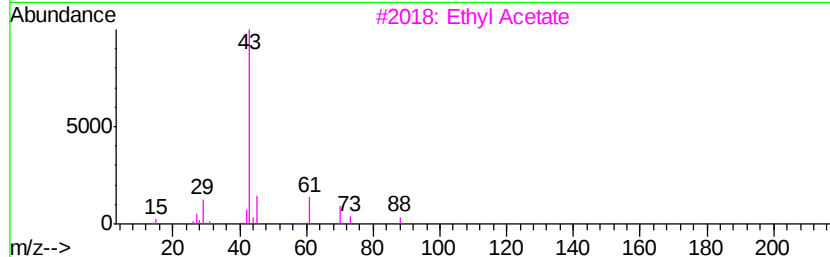
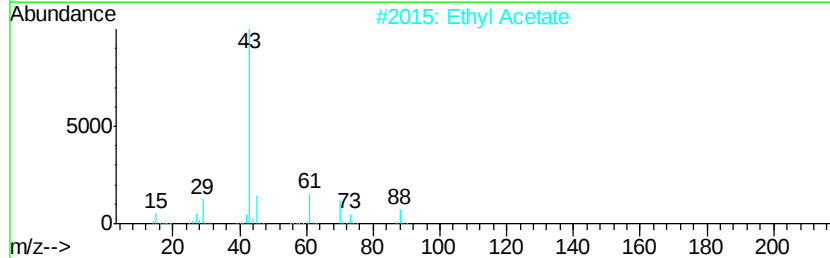
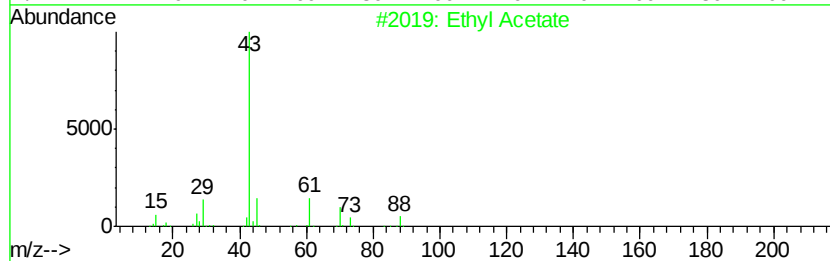
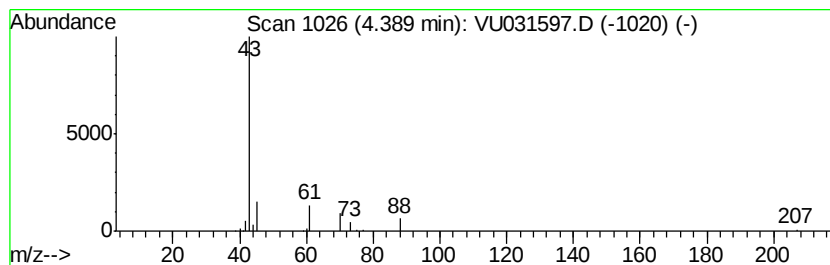
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethyl Acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.39	2.67 ug/L	89386	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethyl Acetate	88	C4H8O2	000141-78-6	86
2		Ethyl Acetate	88	C4H8O2	000141-78-6	86
3		Ethyl Acetate	88	C4H8O2	000141-78-6	80
4		Ethyl Acetate	88	C4H8O2	000141-78-6	59
5		Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	9



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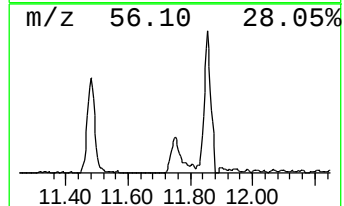
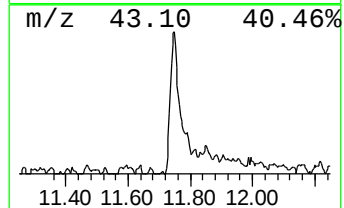
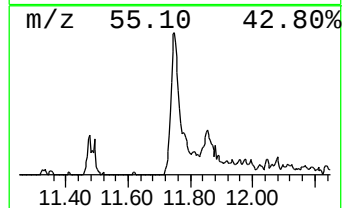
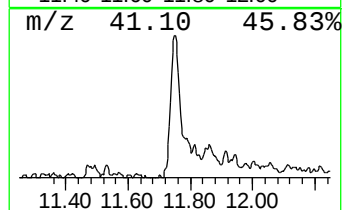
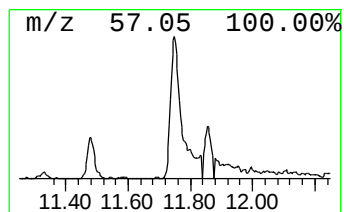
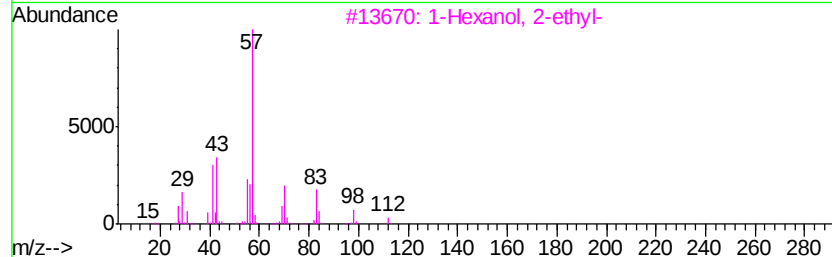
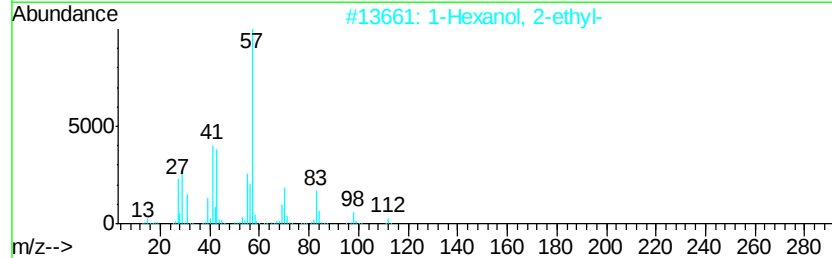
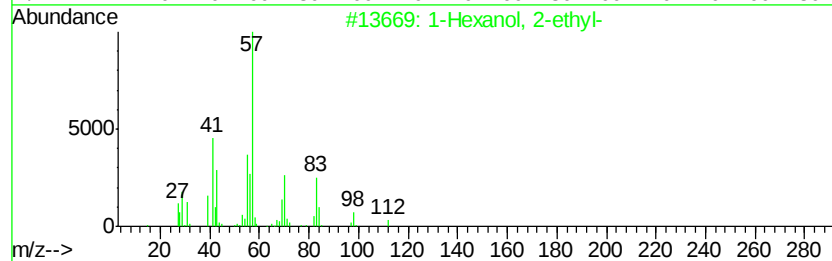
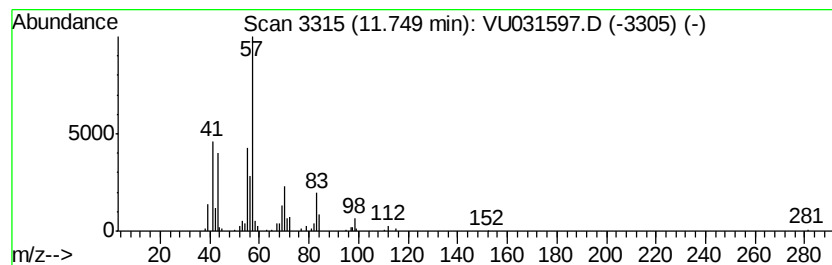
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	4.20 ug/L	135666	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
3		1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
4		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
5		Oxirane, [[(2-ethylhexyl)oxy]met...	186	C11H22O2	002461-15-6	50



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MSVOA_U
ClientSampleId :
C0X09

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042719WMA.M
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
Ethane, 1,1-diflu...	1.18	2.5	ug/L	83733	1	5.88	1672130	50.0
Ethyl Acetate	4.39	2.7	ug/L	89386	1	5.88	1672130	50.0
1-Hexanol, 2-ethyl-	11.75	4.2	ug/L	135666	3	11.48	1613950	50.0