

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU030419\
 Data File : VU029782.D
 Acq On : 04 Mar 2019 14:01
 Operator : JC/SP
 Sample : K1657-13
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DB658

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\SOMULM021519WMA.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	1.183	22	29	45	rVB	139928	136881	9.35%	1.107%
2	1.396	87	95	108	rBV3	232743	269853	18.44%	2.183%
3	1.679	176	183	196	rVB	153668	193782	13.24%	1.568%
4	2.270	359	367	378	rVB	313641	466740	31.89%	3.776%
5	2.531	446	448	449	rBV	451	184	0.01%	0.001%
6	2.637	472	481	482	rBV5	1568	1958	0.13%	0.016%
7	2.820	533	538	546	rBV6	859	1587	0.11%	0.013%
8	2.916	565	568	573	rVB2	468	364	0.02%	0.003%
9	2.965	580	583	584	rBV	287	160	0.01%	0.001%
10	3.045	605	608	611	rBV2	347	264	0.02%	0.002%
11	3.068	612	615	618	rVV	342	191	0.01%	0.002%
12	3.113	626	629	632	rBV3	447	357	0.02%	0.003%
13	3.129	632	634	637	rVB	439	242	0.02%	0.002%
14	3.193	642	654	665	rBV7	4381	10309	0.70%	0.083%
15	3.257	671	674	677	rVB2	544	342	0.02%	0.003%
16	3.293	677	685	686	rBV3	1777	1509	0.10%	0.012%
17	3.347	700	702	705	rBV	215	123	0.01%	0.001%
18	3.363	705	707	713	rVB2	388	362	0.02%	0.003%
19	3.392	713	716	717	rBV	243	163	0.01%	0.001%
20	3.408	717	721	725	rBV6	1132	1163	0.08%	0.009%
21	3.547	759	764	768	rBV2	724	833	0.06%	0.007%
22	3.582	772	775	777	rBV	251	161	0.01%	0.001%
23	3.669	799	802	804	rBV2	225	105	0.01%	0.001%
24	3.685	804	807	808	rBV2	424	216	0.01%	0.002%
25	3.797	839	842	844	rBV3	553	364	0.02%	0.003%
26	3.875	862	866	870	rBV2	306	333	0.02%	0.003%
27	3.920	874	880	884	rVV2	760	839	0.06%	0.007%
28	3.942	884	887	893	rVB2	534	367	0.03%	0.003%
29	4.074	924	928	932	rVB3	504	404	0.03%	0.003%
30	4.093	932	934	936	rBV	244	82	0.01%	0.001%
31	4.109	936	939	942	rBV	490	384	0.03%	0.003%
32	4.174	947	959	983	rBV	138481	365461	24.97%	2.956%
33	4.646	1087	1106	1130	rBV	240907	582436	39.79%	4.711%
34	4.881	1173	1179	1182	rBV5	969	1130	0.08%	0.009%

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 Title : VOC Analysis

35	4.974	1205	1208	1212	rBV2	649	560	0.04%	0.005%
36	5.032	1224	1226	1229	rVB2	462	209	0.01%	0.002%
37	5.051	1229	1232	1233	rBV	289	192	0.01%	0.002%
38	5.125	1253	1255	1257	rBV	534	284	0.02%	0.002%
39	5.138	1257	1259	1262	rVV2	324	248	0.02%	0.002%
40	5.180	1268	1272	1276	rBV2	454	384	0.03%	0.003%
41	5.231	1284	1288	1293	rVB2	644	518	0.04%	0.004%
42	5.251	1293	1294	1297	rBV	213	66	0.00%	0.001%
43	5.338	1297	1321	1355	rBV2	493455	1463677	100.00%	11.840%
44	5.547	1385	1386	1389	rVB2	542	191	0.01%	0.002%
45	5.572	1389	1394	1396	rBV	763	635	0.04%	0.005%
46	5.604	1402	1404	1408	rVB3	880	440	0.03%	0.004%
47	5.730	1440	1443	1445	rBV2	325	246	0.02%	0.002%
48	5.752	1447	1450	1452	rVV	600	330	0.02%	0.003%
49	5.884	1477	1491	1513	rBV	481417	949617	64.88%	7.682%
50	6.087	1552	1554	1556	rBV2	685	376	0.03%	0.003%
51	6.138	1564	1570	1571	rBV2	517	541	0.04%	0.004%
52	6.280	1611	1614	1615	rBV2	489	294	0.02%	0.002%
53	6.328	1615	1629	1655	rVV	322178	658433	44.98%	5.326%
54	6.694	1741	1743	1746	rBV3	274	136	0.01%	0.001%
55	6.807	1775	1778	1781	rBV2	391	245	0.02%	0.002%
56	6.923	1811	1814	1816	rBV2	477	297	0.02%	0.002%
57	6.993	1832	1836	1838	rBV	572	364	0.02%	0.003%
58	7.035	1846	1849	1853	rBV2	471	432	0.03%	0.003%
59	7.058	1853	1856	1858	rBV2	346	240	0.02%	0.002%
60	7.090	1863	1866	1867	rBV	278	171	0.01%	0.001%
61	7.132	1877	1879	1881	rBV	346	215	0.01%	0.002%
62	7.225	1896	1908	1927	rBV	184135	332072	22.69%	2.686%
63	7.473	1979	1985	1988	rBV5	1105	1266	0.09%	0.010%
64	7.563	1999	2013	2030	rBV	687736	1190628	81.34%	9.631%
65	7.849	2091	2102	2127	rBV	127945	225510	15.41%	1.824%
66	8.119	2183	2186	2188	rBV	447	315	0.02%	0.003%
67	8.177	2193	2204	2214	rVV2	17595	31613	2.16%	0.256%
68	8.309	2234	2245	2283	rBV	491545	879892	60.12%	7.118%
69	8.463	2285	2293	2313	rVB3	50462	88630	6.06%	0.717%
70	8.701	2365	2367	2375	rVB2	432	405	0.03%	0.003%
71	8.765	2381	2387	2389	rBV	627	656	0.04%	0.005%

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72	8.797	2391	2397	2403	rVV4	859	1136	0.08%	0.009%
73	8.903	2428	2430	2431	rBV	311	149	0.01%	0.001%
74	8.939	2438	2441	2446	rBV2	475	519	0.04%	0.004%
75	8.981	2451	2454	2458	rVB	730	494	0.03%	0.004%
76	9.003	2458	2461	2464	rBV2	403	372	0.03%	0.003%
77	9.019	2464	2466	2469	rBV3	427	266	0.02%	0.002%
78	9.087	2474	2487	2525	rBV	702651	1183159	80.83%	9.571%
79	9.318	2556	2559	2561	rBV3	650	357	0.02%	0.003%
80	9.376	2570	2577	2587	rBV3	4813	7208	0.49%	0.058%
81	9.456	2597	2602	2605	rVB3	365	357	0.02%	0.003%
82	9.479	2606	2609	2611	rBV	404	288	0.02%	0.002%
83	9.514	2617	2620	2622	rBV2	544	362	0.02%	0.003%
84	9.704	2672	2679	2682	rBV5	2632	3493	0.24%	0.028%
85	10.038	2774	2783	2796	rVB6	2553	4834	0.33%	0.039%
86	10.164	2811	2822	2825	rBV4	1109	1744	0.12%	0.014%
87	10.260	2849	2852	2853	rBV2	358	183	0.01%	0.001%
88	10.296	2860	2863	2866	rBV2	455	309	0.02%	0.002%
89	10.350	2877	2880	2882	rBV	541	306	0.02%	0.002%
90	10.363	2882	2884	2885	rBV	335	138	0.01%	0.001%
91	10.427	2893	2904	2921	rBV	530333	845895	57.79%	6.843%
92	10.604	2950	2959	2969	rVB2	19309	32290	2.21%	0.261%
93	10.903	3049	3052	3056	rBV4	480	449	0.03%	0.004%
94	11.234	3153	3155	3158	rBV2	604	471	0.03%	0.004%
95	11.479	3220	3231	3255	rBV	741938	1189684	81.28%	9.624%
96	11.749	3307	3315	3334	rBV	21700	45012	3.08%	0.364%
97	11.858	3337	3349	3368	rVV	707747	1169888	79.93%	9.464%
98	12.900	3665	3673	3678	rBV6	1471	2670	0.18%	0.022%

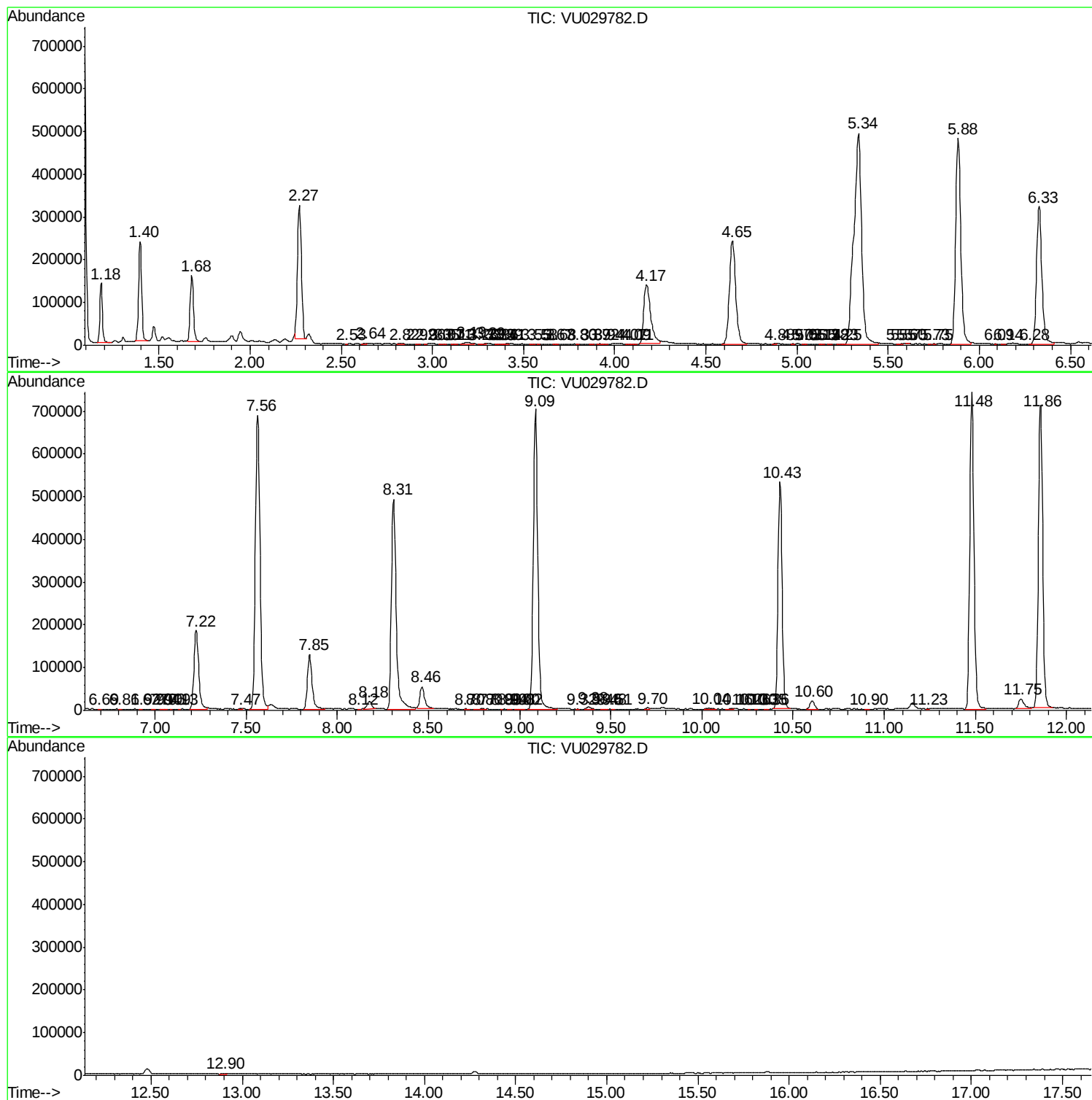
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM021519WMA.M
Quant Title : VOC Analysis

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



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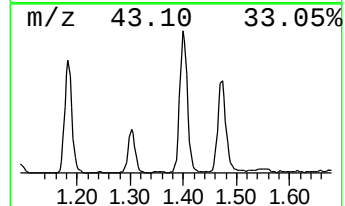
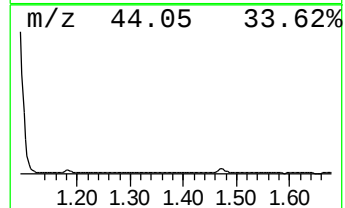
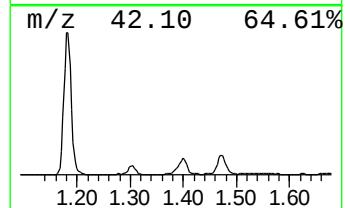
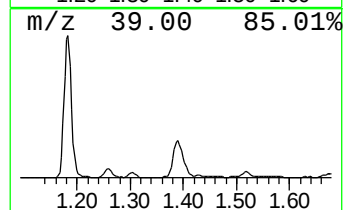
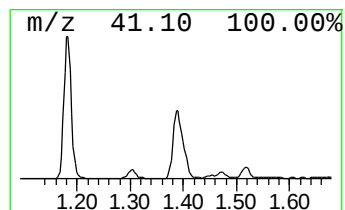
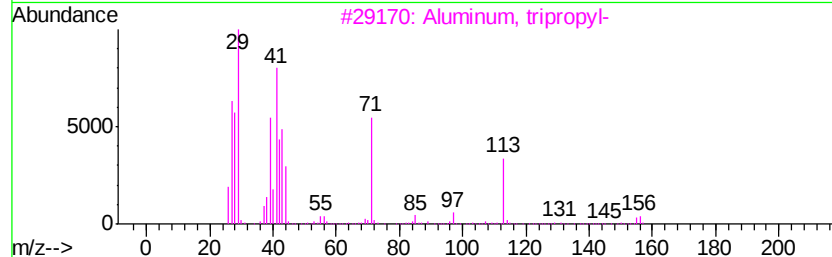
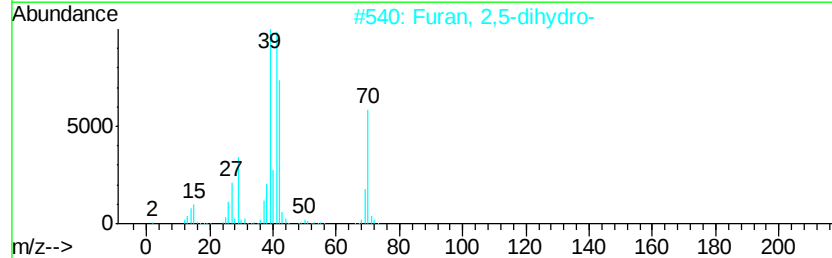
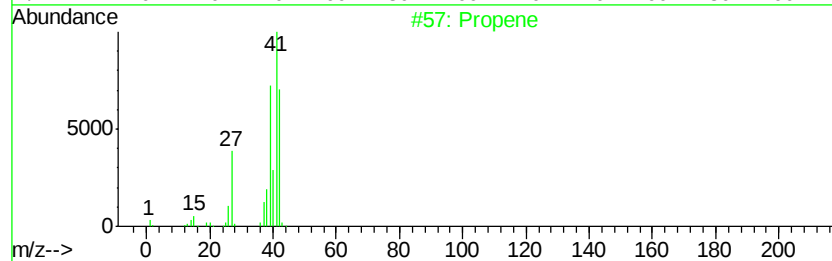
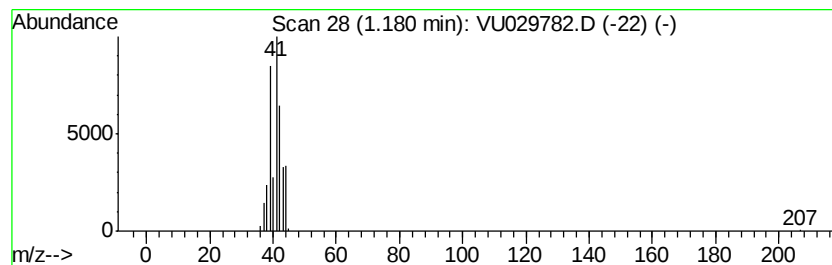
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM021519WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Cyclic1.18 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.18	7.21 ug/L	136881	1,4-Difluorobenzene	5.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propene	42	C3H6	000115-07-1	90
2		Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	83
3		Aluminum, tripropyl-	156	C9H21Al	000102-67-0	83
4		2-Butenal, (E)-	70	C4H6O	000123-73-9	78
5		Pyrimidin-4(3H)-one, 3-amino-2,6...	139	C6H9N3O	093098-74-9	78



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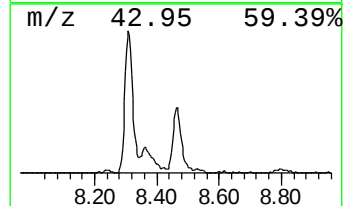
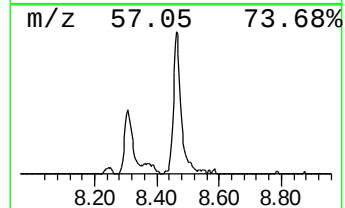
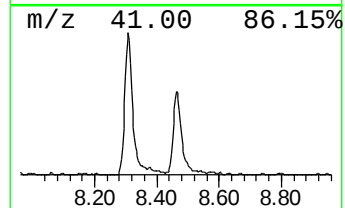
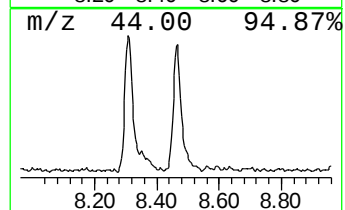
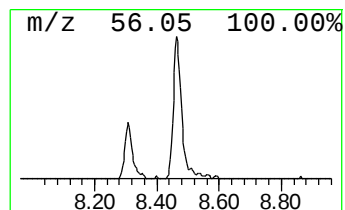
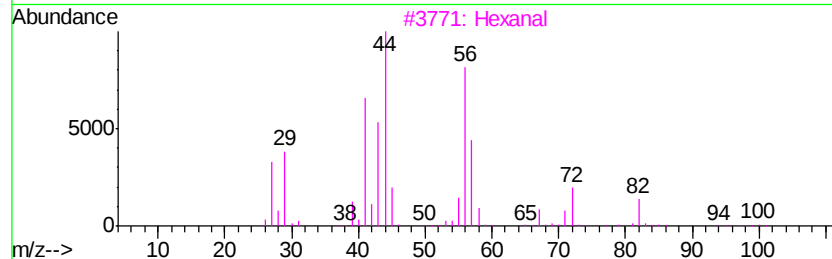
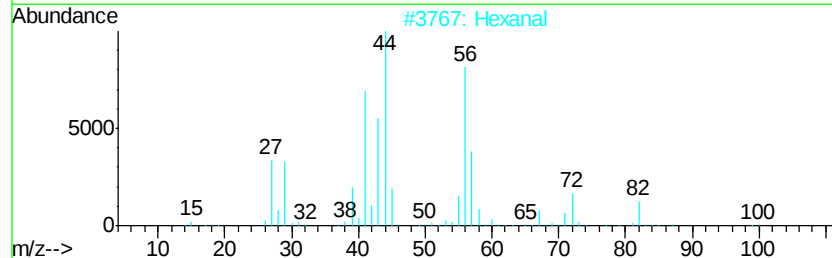
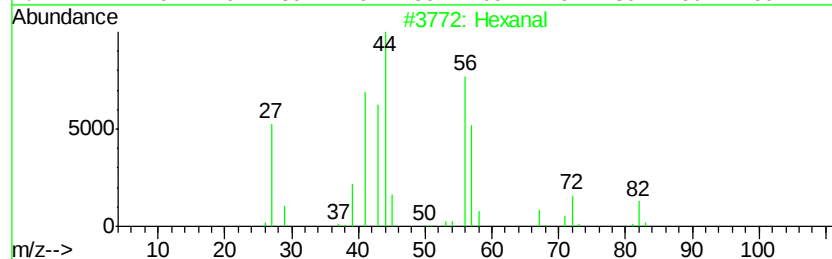
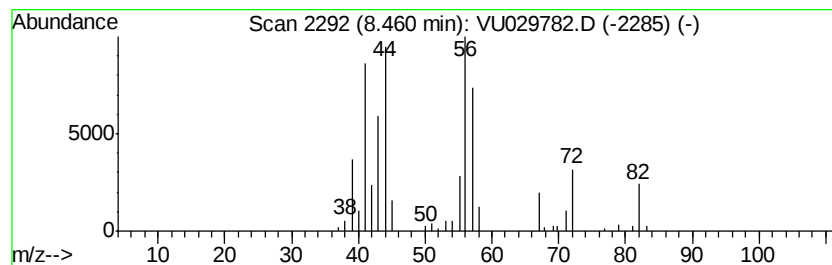
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Quant Title : VOC Analysis

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TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.46	3.75 ug/L	88630	Chlorobenzene-d5	9.09

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal		100	C6H12O	000066-25-1	78
2	Hexanal		100	C6H12O	000066-25-1	78
3	Hexanal		100	C6H12O	000066-25-1	56
4	Hexanal		100	C6H12O	000066-25-1	38
5	Glutaraldehyde		100	C5H8O2	000111-30-8	32



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: Cyc...	1.18	7.2	ug/L	136881	1	5.88	949617	50.0
Hexanal	8.46	3.8	ug/L	88630	2	9.09	1183160	50.0