

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU042919\
 Data File : VU031598.D
 Acq On : 29 Apr 2019 19:47
 Operator : JC/SP
 Sample : K2536-22
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0X10

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	35	rVB2	53769	51903	0.29%	0.115%
2	1.293	59	63	68	rVB2	18162	16085	0.09%	0.036%
3	1.396	88	95	106	rVB	420033	449457	2.50%	0.995%
4	1.679	176	183	198	rVB	361641	443979	2.47%	0.982%
5	1.884	238	247	263	rVB	353384	495598	2.76%	1.097%
6	2.270	356	367	379	rBV	725665	1103211	6.15%	2.441%
7	2.338	380	388	404	rVB2	58077	128491	0.72%	0.284%
8	2.428	414	416	419	rBV4	1467	1044	0.01%	0.002%
9	2.804	529	533	534	rBV	2016	1386	0.01%	0.003%
10	2.839	534	544	551	rVV6	6393	13124	0.07%	0.029%
11	2.936	571	574	578	rBV3	1399	1047	0.01%	0.002%
12	2.978	578	587	588	rBV5	1942	2224	0.01%	0.005%
13	3.277	675	680	681	rBV3	1188	899	0.01%	0.002%
14	3.431	725	728	732	rBV3	1349	957	0.01%	0.002%
15	3.495	745	748	753	rBV3	1570	1097	0.01%	0.002%
16	3.566	767	770	772	rBV3	1747	911	0.01%	0.002%
17	3.595	776	779	786	rVB5	975	1018	0.01%	0.002%
18	3.640	790	793	798	rVB2	943	982	0.01%	0.002%
19	3.704	809	813	818	rVB2	1432	1404	0.01%	0.003%
20	3.746	822	826	829	rBV2	1708	1379	0.01%	0.003%
21	3.888	865	870	875	rVB3	1371	1381	0.01%	0.003%
22	3.952	887	890	894	rVB2	1657	1280	0.01%	0.003%
23	4.000	894	905	908	rBV6	1837	2979	0.02%	0.007%
24	4.068	921	926	929	rBV2	932	988	0.01%	0.002%
25	4.187	949	963	1007	rBV	309200	1029941	5.74%	2.279%
26	4.389	1020	1026	1053	rVB3	31564	87446	0.49%	0.194%
27	4.643	1088	1105	1133	rBV2	534156	1289958	7.19%	2.855%
28	5.132	1243	1257	1270	rBV5	7169	16347	0.09%	0.036%
29	5.199	1275	1278	1284	rVB5	1371	1168	0.01%	0.003%
30	5.334	1296	1320	1362	rBV2	1071939	3303916	18.40%	7.311%
31	5.585	1396	1398	1403	rBV4	1802	1151	0.01%	0.003%
32	5.743	1444	1447	1448	rBV3	2068	1200	0.01%	0.003%
33	5.794	1460	1463	1467	rVB3	2459	1440	0.01%	0.003%
34	5.881	1476	1490	1520	rBV	811563	1696737	9.45%	3.755%

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 Title : VOC Analysis

35	6.093	1552	1556	1564	rBV7	2557	3076	0.02%	0.007%
36	6.180	1567	1583	1617	rBV	9191889	17951590	100.00%	39.725%
37	6.325	1618	1628	1656	rVB	758923	1609765	8.97%	3.562%
38	6.820	1779	1782	1787	rBV4	1946	1808	0.01%	0.004%
39	6.974	1826	1830	1834	rVB4	1267	1215	0.01%	0.003%
40	7.045	1847	1852	1856	rBV5	1168	1406	0.01%	0.003%
41	7.116	1871	1874	1876	rBV4	1886	1375	0.01%	0.003%
42	7.141	1880	1882	1886	rVB	1749	1135	0.01%	0.003%
43	7.167	1886	1890	1893	rBV3	1705	1329	0.01%	0.003%
44	7.225	1894	1908	1927	rBV	366592	687960	3.83%	1.522%
45	7.563	2000	2013	2057	rBV	1269237	2391682	13.32%	5.292%
46	7.801	2085	2087	2090	rVB3	2388	1279	0.01%	0.003%
47	7.849	2091	2102	2123	rBV2	248606	454444	2.53%	1.006%
48	8.074	2167	2172	2183	rVB9	3894	5320	0.03%	0.012%
49	8.174	2193	2203	2205	rBV7	7047	9572	0.05%	0.021%
50	8.222	2206	2218	2236	rVV	1412984	2496651	13.91%	5.525%
51	8.309	2236	2245	2284	rVB	1029633	2077655	11.57%	4.598%
52	8.710	2367	2370	2372	rBV3	1457	1115	0.01%	0.002%
53	8.881	2420	2423	2429	rVB6	1860	1654	0.01%	0.004%
54	8.955	2442	2446	2451	rBV6	1008	907	0.01%	0.002%
55	9.087	2474	2487	2526	rBV	1213417	2165421	12.06%	4.792%
56	9.469	2602	2606	2614	rVB5	2518	2798	0.02%	0.006%
57	9.601	2644	2647	2652	rVB5	1134	1009	0.01%	0.002%
58	9.646	2658	2661	2663	rBV2	1911	1292	0.01%	0.003%
59	9.688	2670	2674	2679	rVB5	1354	1220	0.01%	0.003%
60	9.752	2691	2694	2697	rBV2	1323	884	0.00%	0.002%
61	9.794	2704	2707	2710	rBV3	1370	1242	0.01%	0.003%
62	9.858	2723	2727	2730	rBV4	1562	1236	0.01%	0.003%
63	9.907	2739	2742	2745	rVB3	1595	973	0.01%	0.002%
64	9.939	2749	2752	2755	rVB3	1721	1122	0.01%	0.002%
65	9.961	2755	2759	2760	rBV3	1370	863	0.00%	0.002%
66	9.993	2765	2769	2772	rBV4	1267	1003	0.01%	0.002%
67	10.051	2785	2787	2790	rVB2	1928	933	0.01%	0.002%
68	10.132	2809	2812	2816	rBV3	1588	1226	0.01%	0.003%
69	10.209	2833	2836	2837	rBV2	1966	1119	0.01%	0.002%
70	10.427	2891	2904	2928	rVV	942515	1527207	8.51%	3.380%
71	10.604	2952	2959	2967	rVB5	6914	10247	0.06%	0.023%

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72	10.649	2971	2973	2979	rVB5	2184	2022	0.01%	0.004%
73	10.694	2980	2987	2992	rBV5	2313	3245	0.02%	0.007%
74	10.730	2995	2998	3003	rVV5	1549	1446	0.01%	0.003%
75	10.804	3019	3021	3026	rBV3	1400	974	0.01%	0.002%
76	10.961	3066	3070	3075	rVB4	1495	1571	0.01%	0.003%
77	11.048	3092	3097	3103	rVV5	2034	2473	0.01%	0.005%
78	11.083	3106	3108	3113	rVB3	2633	1852	0.01%	0.004%
79	11.119	3116	3119	3121	rBV3	1504	836	0.00%	0.002%
80	11.148	3121	3128	3133	rBV6	1432	2267	0.01%	0.005%
81	11.202	3141	3145	3151	rBV3	1195	1659	0.01%	0.004%
82	11.286	3167	3171	3175	rBV3	1102	1145	0.01%	0.003%
83	11.353	3189	3192	3196	rVB4	1657	1470	0.01%	0.003%
84	11.379	3196	3200	3203	rBV4	1056	932	0.01%	0.002%
85	11.479	3219	3231	3255	rBV	1012719	1640114	9.14%	3.629%
86	11.749	3306	3315	3329	rBV2	47652	101632	0.57%	0.225%
87	11.855	3337	3348	3372	rBV	1101726	1830473	10.20%	4.051%
88	12.312	3488	3490	3497	rVB6	3056	2248	0.01%	0.005%
89	12.392	3513	3515	3518	rBV5	1593	1087	0.01%	0.002%
90	12.450	3530	3533	3537	rVB3	2113	1443	0.01%	0.003%
91	12.479	3537	3542	3549	rVB6	3315	4359	0.02%	0.010%
92	12.521	3553	3555	3559	rBV3	2118	1557	0.01%	0.003%
93	12.624	3584	3587	3590	rBV2	1790	1271	0.01%	0.003%
94	12.784	3635	3637	3642	rVB3	2286	1668	0.01%	0.004%
95	12.942	3683	3686	3689	rBV3	1439	1242	0.01%	0.003%
96	13.312	3795	3801	3805	rBV7	2413	2651	0.01%	0.006%
97	13.874	3974	3976	3980	rVB2	2171	1432	0.01%	0.003%
98	13.897	3980	3983	3989	rBV4	1811	1929	0.01%	0.004%
99	14.128	4052	4055	4057	rBV3	1676	1334	0.01%	0.003%
100	14.849	4277	4279	4282	rBV4	1447	860	0.00%	0.002%

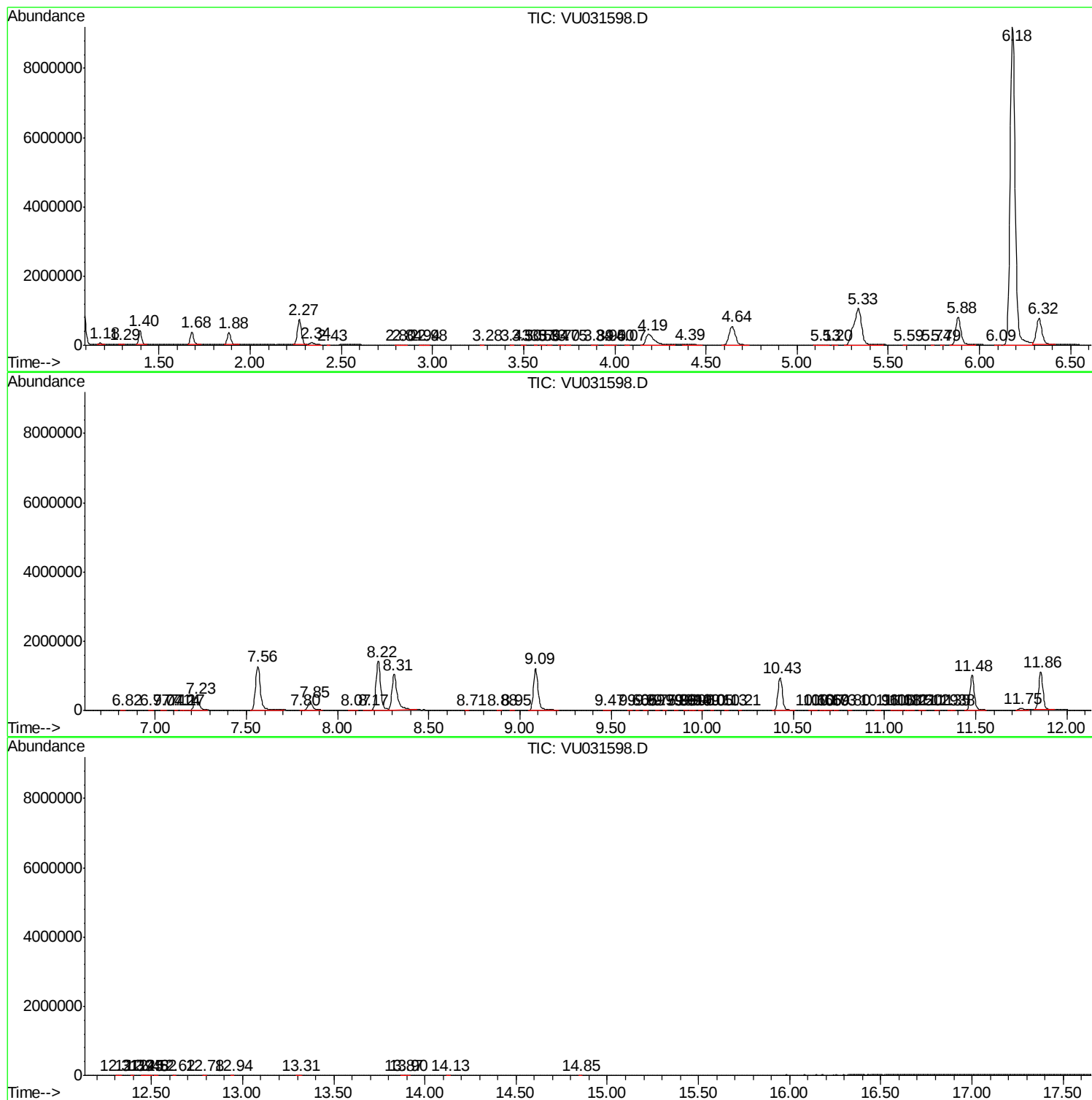
Sum of corrected areas: 45190053

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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



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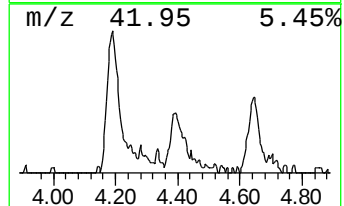
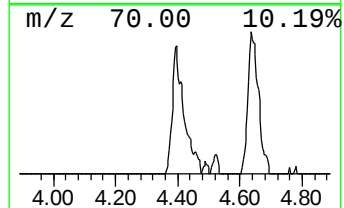
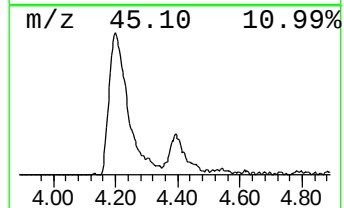
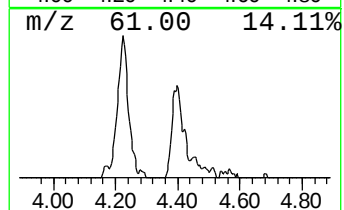
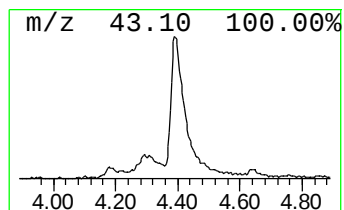
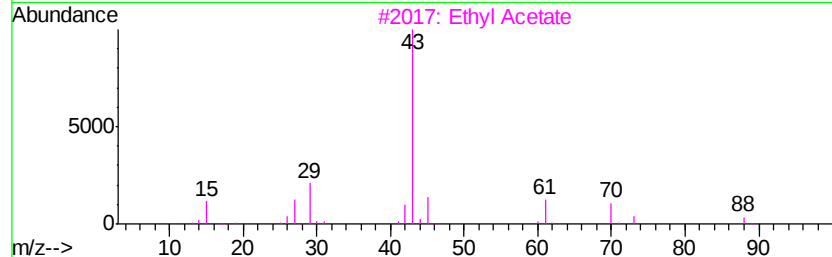
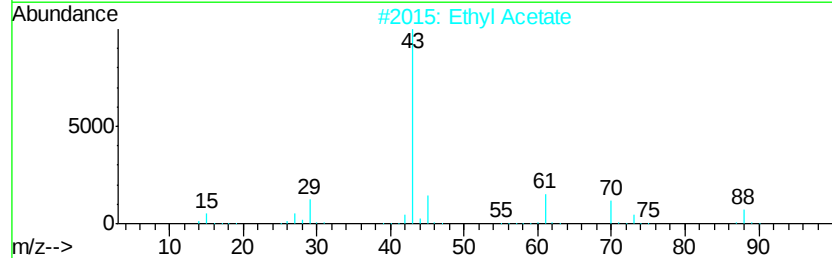
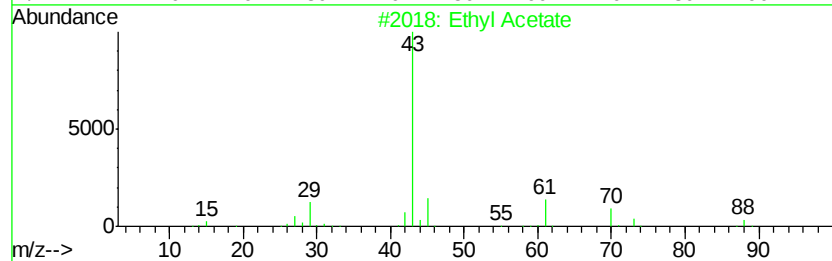
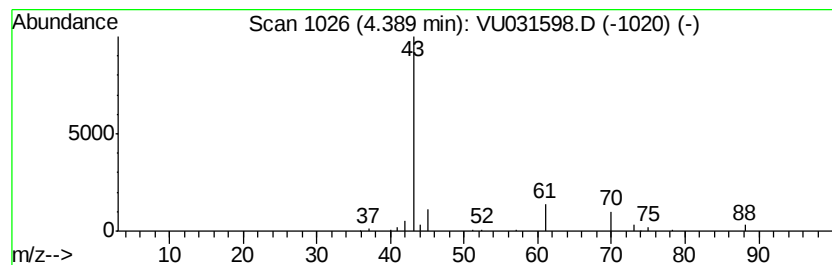
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM042719WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Ethyl Acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.39	2.58 ug/L	87446	1,4-Difluorobenzene	5.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl Acetate	88	C4H8O2	000141-78-6	86
2			Ethyl Acetate	88	C4H8O2	000141-78-6	64
3			Ethyl Acetate	88	C4H8O2	000141-78-6	59
4			Ethyl Acetate	88	C4H8O2	000141-78-6	59
5			CH3C(O)CH2CH2OH	88	C4H8O2	000590-90-9	9



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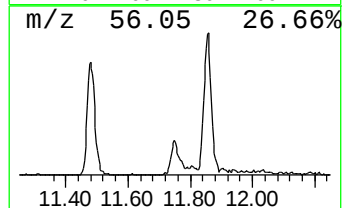
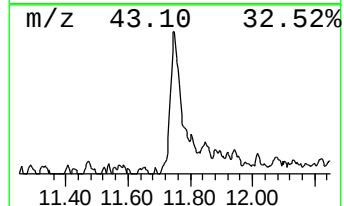
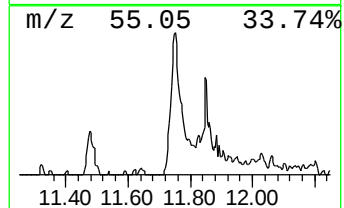
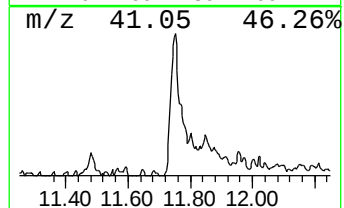
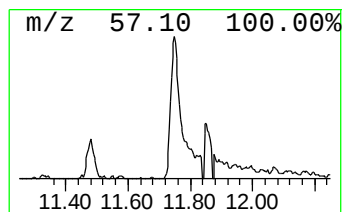
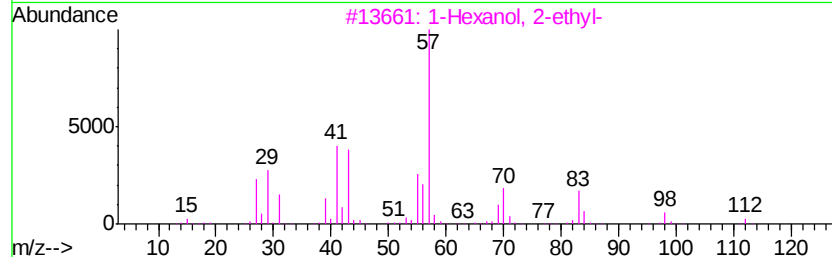
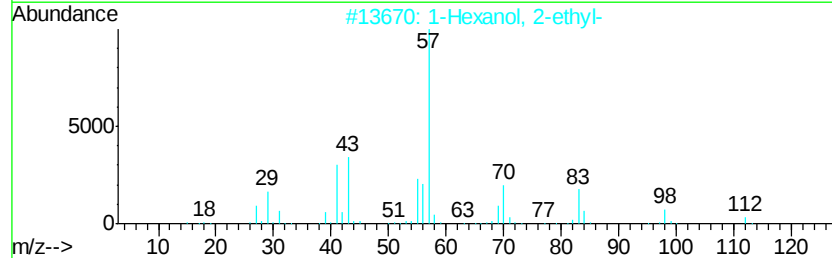
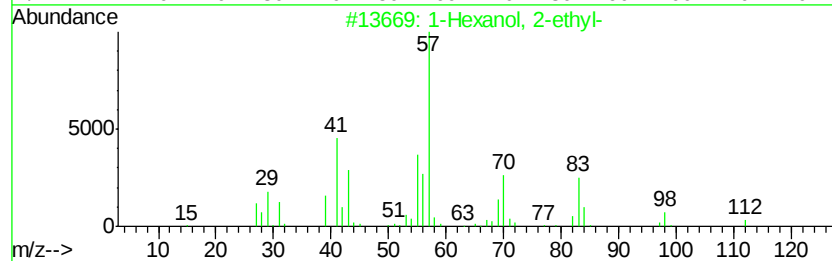
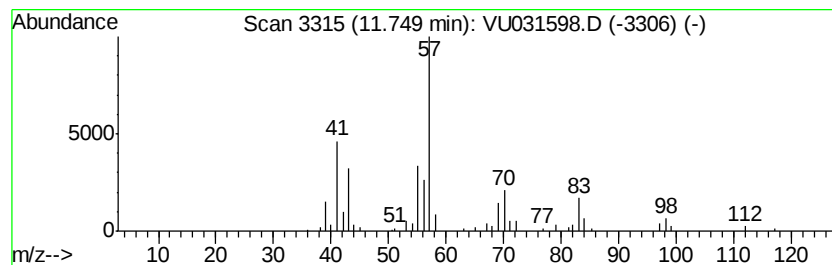
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Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	3.10 ug/L	101632	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7 78
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7 72
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7 64
4	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2 64
5	Heptyl isobutyl carbonate	216	C12H24O3	959068-08-7 64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethyl Acetate	4.39	2.6	ug/L	87446	1	5.88	1696740	50.0
1-Hexanol, 2-ethyl-	11.75	3.1	ug/L	101632	3	11.48	1640110	50.0