

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU051120\
 Data File : VU038108.D
 Acq On : 11 May 2020 15:58
 Operator : JC/MD
 Sample : L2578-01DL 20X
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFSE9DL

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\SOMULM043020WMA.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	1.613	77	85	97	rBV	309896	340036	13.08%	1.385%
2	1.929	175	183	196	rVB	281068	362714	13.96%	1.477%
3	2.594	378	390	407	rBV2	486809	820589	31.57%	3.341%
4	2.803	443	455	460	rBV3	3705	7439	0.29%	0.030%
5	2.903	484	486	490	rVB3	632	486	0.02%	0.002%
6	2.925	490	493	497	rBV4	433	390	0.02%	0.002%
7	3.157	563	565	570	rVB2	729	510	0.02%	0.002%
8	3.218	570	584	600	rVB3	8157	19809	0.76%	0.081%
9	3.314	611	614	620	rBV2	538	598	0.02%	0.002%
10	3.578	689	696	699	rVB4	585	807	0.03%	0.003%
11	3.639	713	715	720	rVB3	829	640	0.02%	0.003%
12	3.909	782	799	819	rVB	175032	416308	16.02%	1.695%
13	3.996	824	826	827	rBV2	845	403	0.02%	0.002%
14	4.041	828	840	850	rVV3	5174	12195	0.47%	0.050%
15	4.076	850	851	856	rVB2	837	547	0.02%	0.002%
16	4.276	906	913	918	rVB2	548	746	0.03%	0.003%
17	4.597	1011	1013	1017	rVB	648	463	0.02%	0.002%
18	4.662	1017	1033	1063	rBV	341203	850584	32.73%	3.463%
19	4.954	1118	1124	1127	rVB3	821	851	0.03%	0.003%
20	4.977	1127	1131	1139	rBV4	719	941	0.04%	0.004%
21	5.102	1152	1170	1192	rVV	450414	988500	38.04%	4.025%
22	5.240	1212	1213	1219	rVB3	719	579	0.02%	0.002%
23	5.353	1230	1248	1273	rVV	743668	1674051	64.41%	6.817%
24	5.594	1318	1323	1327	rBV5	402	415	0.02%	0.002%
25	5.668	1343	1346	1349	rBV3	623	423	0.02%	0.002%
26	5.758	1351	1374	1402	rBV2	966449	2598902	100.00%	10.582%
27	6.022	1453	1456	1460	rBV3	698	546	0.02%	0.002%
28	6.102	1479	1481	1485	rVB4	728	419	0.02%	0.002%
29	6.141	1489	1493	1501	rVB6	1289	1312	0.05%	0.005%
30	6.192	1506	1509	1513	rVB3	646	421	0.02%	0.002%
31	6.215	1513	1516	1520	rBV4	666	492	0.02%	0.002%
32	6.279	1520	1536	1572	rBV	916718	1757494	67.62%	7.156%
33	6.446	1585	1588	1590	rBV3	570	452	0.02%	0.002%
34	6.559	1612	1623	1639	rBV6	9778	21194	0.82%	0.086%

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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM043020WMA.M
 Title : VOC Analysis

35	6.719	1656	1673	1698	rBV	625151	1211640	46.62%	4.934%
36	6.829	1705	1707	1709	rBV2	1057	467	0.02%	0.002%
37	6.944	1730	1743	1754	rBV3	21696	42406	1.63%	0.173%
38	7.086	1783	1787	1791	rVV2	539	423	0.02%	0.002%
39	7.208	1817	1825	1838	rVB2	6115	10042	0.39%	0.041%
40	7.362	1861	1873	1887	rVB3	19146	36089	1.39%	0.147%
41	7.440	1893	1897	1903	rVB3	581	693	0.03%	0.003%
42	7.536	1915	1927	1933	rBV2	29199	48308	1.86%	0.197%
43	7.591	1933	1944	1963	rVB	346831	601074	23.13%	2.448%
44	7.739	1971	1990	2003	rVB6	19250	42323	1.63%	0.172%
45	7.819	2010	2015	2023	rVB6	2491	3173	0.12%	0.013%
46	7.922	2031	2047	2080	rBV	1146552	2059177	79.23%	8.385%
47	8.086	2092	2098	2105	rVV3	1343	1561	0.06%	0.006%
48	8.198	2118	2133	2148	rBV	242226	401513	15.45%	1.635%
49	8.272	2154	2156	2160	rVB3	813	412	0.02%	0.002%
50	8.395	2189	2194	2196	rBV2	652	550	0.02%	0.002%
51	8.417	2196	2201	2203	rBV4	651	425	0.02%	0.002%
52	8.488	2219	2223	2224	rBV	687	485	0.02%	0.002%
53	8.526	2232	2235	2243	rBV3	506	546	0.02%	0.002%
54	8.571	2243	2249	2260	rBV7	956	1567	0.06%	0.006%
55	8.652	2260	2274	2317	rBV	960387	1766175	67.96%	7.192%
56	8.938	2360	2363	2366	rBV2	632	470	0.02%	0.002%
57	9.038	2391	2394	2400	rVV4	504	478	0.02%	0.002%
58	9.070	2400	2404	2410	rVB3	566	610	0.02%	0.002%
59	9.176	2429	2437	2438	rBV	947	995	0.04%	0.004%
60	9.247	2456	2459	2464	rBV2	647	539	0.02%	0.002%
61	9.279	2466	2469	2473	rVB2	661	490	0.02%	0.002%
62	9.436	2503	2518	2541	rBV	1298043	2210361	85.05%	9.000%
63	9.581	2557	2563	2564	rBV3	590	628	0.02%	0.003%
64	9.616	2571	2574	2581	rVB4	857	713	0.03%	0.003%
65	9.652	2581	2585	2592	rVB5	817	914	0.04%	0.004%
66	9.713	2600	2604	2607	rVV4	1199	1112	0.04%	0.005%
67	9.764	2616	2620	2622	rBV3	432	407	0.02%	0.002%
68	10.057	2707	2711	2718	rVB2	584	564	0.02%	0.002%
69	10.131	2732	2734	2737	rVB2	671	391	0.02%	0.002%
70	10.272	2766	2778	2796	rBV	145402	263756	10.15%	1.074%
71	10.488	2839	2845	2846	rBV3	1012	863	0.03%	0.004%

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72	10.558	2860	2867	2876	rVB4	5425	7428	0.29%	0.030%
73	10.665	2898	2900	2910	rVB5	1954	2327	0.09%	0.009%
74	10.771	2917	2933	2951	rBV	874024	1386108	53.33%	5.644%
75	10.896	2968	2972	2983	rVB	2750	4224	0.16%	0.017%
76	10.944	2983	2987	2990	rBV3	1297	1054	0.04%	0.004%
77	10.996	2996	3003	3005	rBV3	1799	1879	0.07%	0.008%
78	11.044	3005	3018	3037	rVV	242517	409460	15.76%	1.667%
79	11.128	3037	3044	3053	rVV5	4674	6962	0.27%	0.028%
80	11.169	3053	3057	3062	rVV6	948	872	0.03%	0.004%
81	11.205	3062	3068	3075	rVV5	3515	4449	0.17%	0.018%
82	11.247	3075	3081	3090	rVB6	2202	3163	0.12%	0.013%
83	11.343	3107	3111	3118	rVB3	1956	1920	0.07%	0.008%
84	11.481	3144	3154	3164	rBV6	1782	3275	0.13%	0.013%
85	11.642	3198	3204	3210	rBV7	1322	2097	0.08%	0.009%
86	11.822	3246	3260	3277	rBV	1391150	2173826	83.64%	8.852%
87	12.105	3339	3348	3356	rVB6	8575	13635	0.52%	0.056%
88	12.205	3365	3379	3402	rBV	1193518	1929852	74.26%	7.858%
89	12.346	3420	3423	3426	rBV3	627	469	0.02%	0.002%
90	12.407	3439	3442	3445	rBV2	693	463	0.02%	0.002%
91	12.571	3490	3493	3495	rBV2	674	521	0.02%	0.002%
92	12.960	3610	3614	3617	rVB3	1151	737	0.03%	0.003%
93	13.169	3675	3679	3684	rBV3	1033	653	0.03%	0.003%
94	13.217	3690	3694	3695	rBV	683	453	0.02%	0.002%
95	13.478	3772	3775	3779	rBV	752	432	0.02%	0.002%
96	13.758	3857	3862	3864	rBV2	892	905	0.03%	0.004%
97	13.870	3894	3897	3901	rBV4	1183	885	0.03%	0.004%
98	13.967	3924	3927	3931	rBV3	1013	865	0.03%	0.004%
99	13.992	3933	3935	3940	rVB2	742	479	0.02%	0.002%
100	14.118	3965	3974	3984	rBV5	2874	4677	0.18%	0.019%

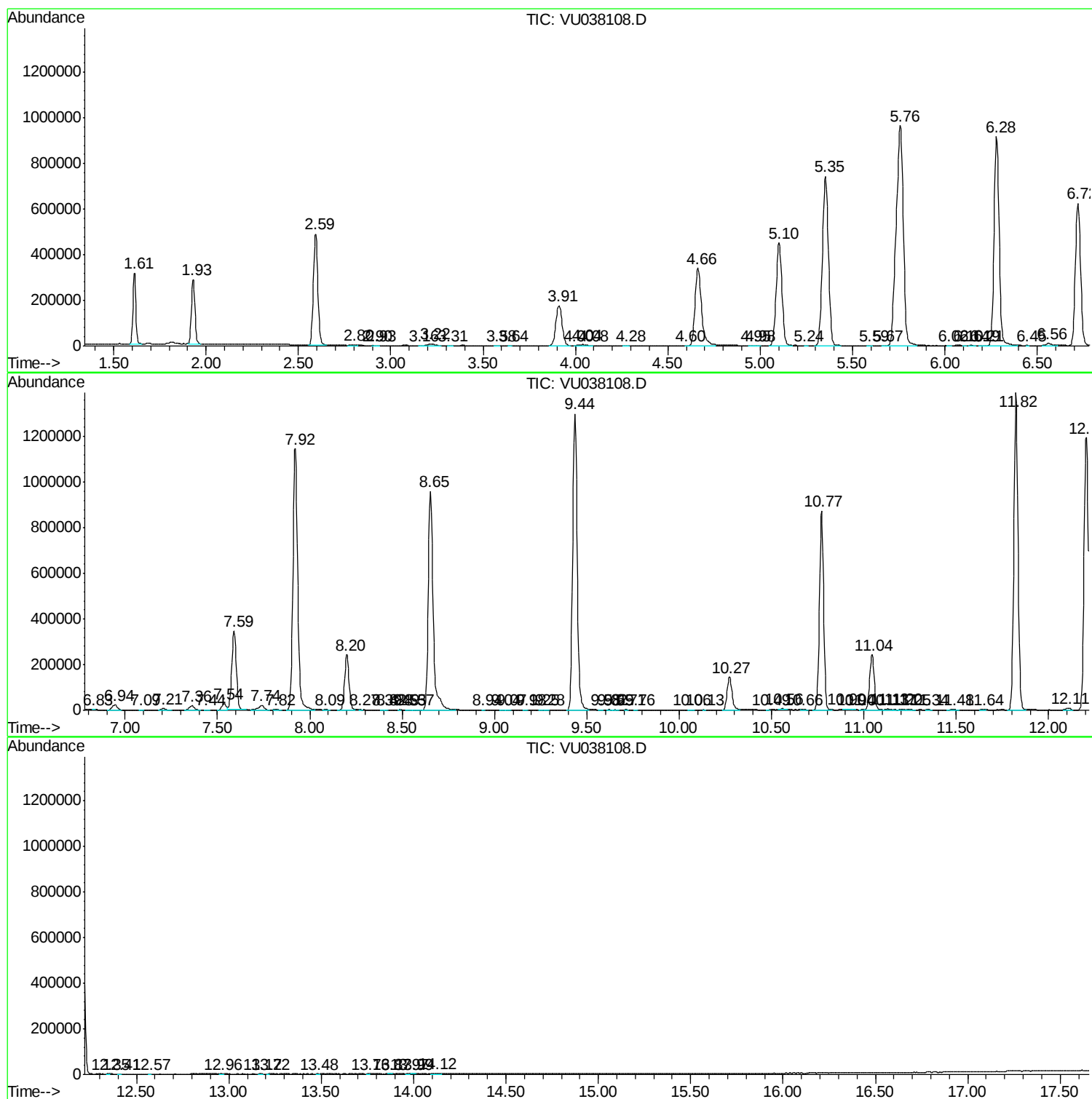
Sum of corrected areas: 24558666

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM043020WMA.M
Quant Title : VOC Analysis

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



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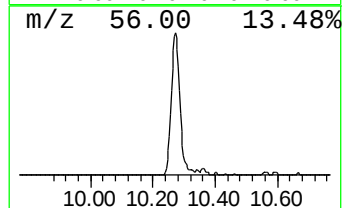
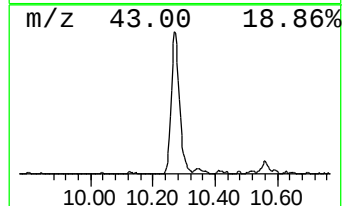
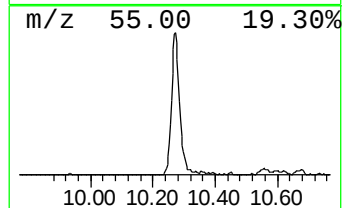
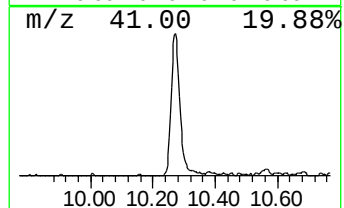
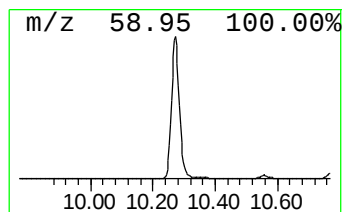
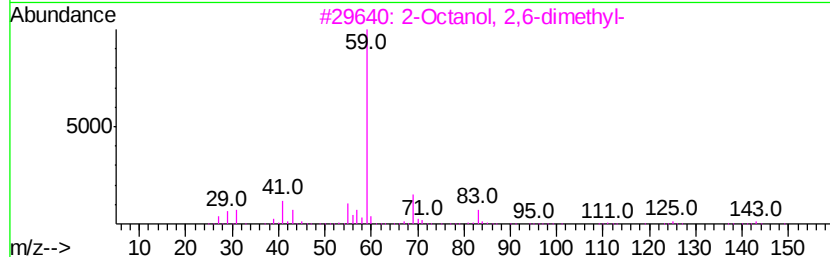
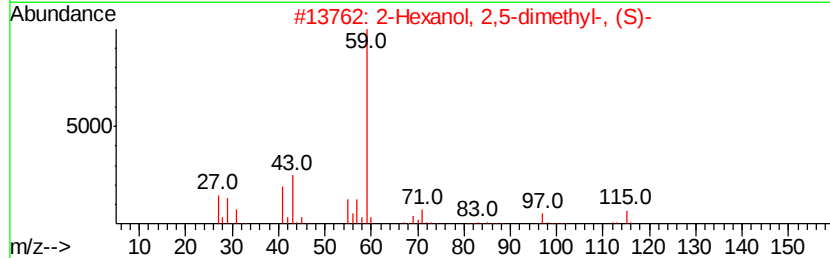
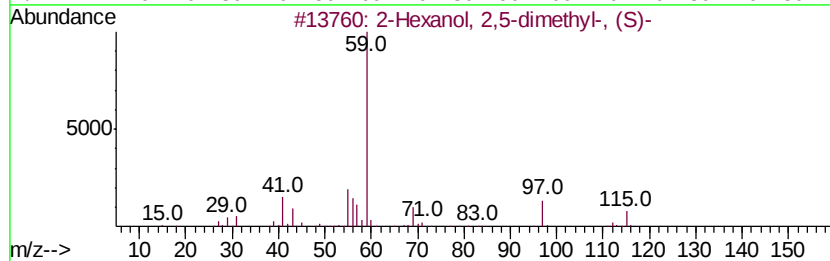
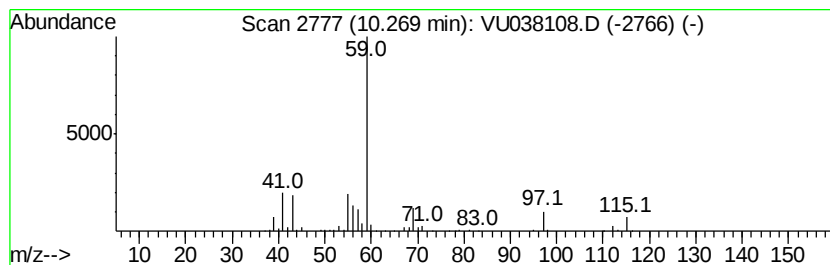
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM043020WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 2-Hexanol, 2,5-dimethyl-, (S)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.27	5.97 ug/L	263756	Chlorobenzene-d5	9.44

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	90
2		2-Hexanol, 2,5-dimethyl-, (S)-	130	C8H18O	003730-60-7	78
3		2-Octanol, 2,6-dimethyl-	158	C10H22O	018479-57-7	50
4		2-Hexanol, methyl ether	116	C7H16O	1000333-92-0	45
5		2-Hydroxy-2,4-dimethyl-3-pentanone	130	C7H14O2	003212-67-7	45



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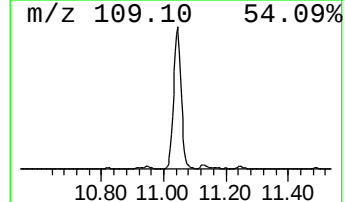
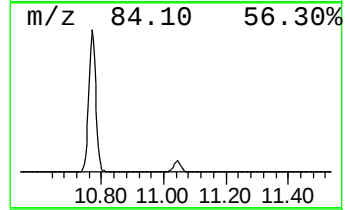
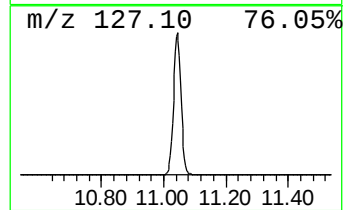
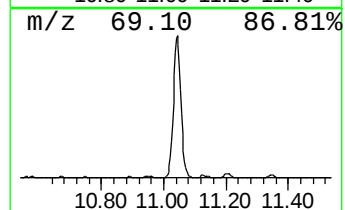
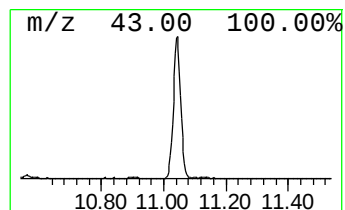
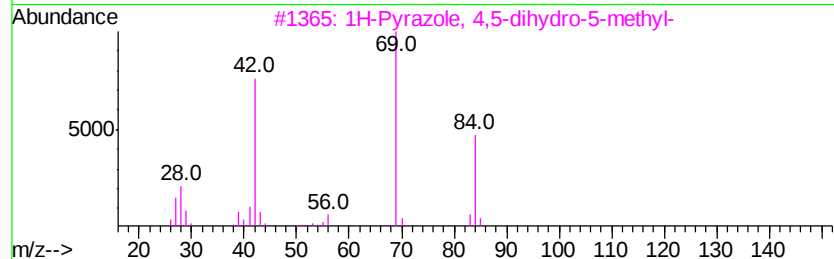
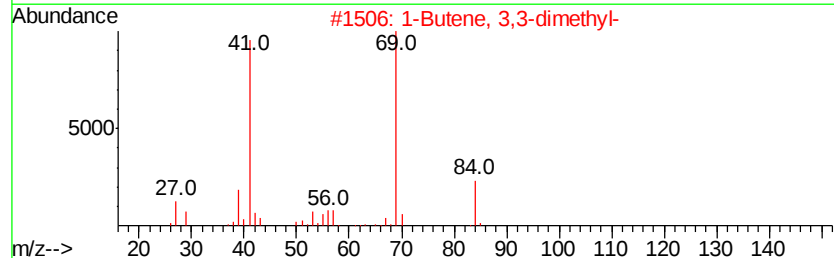
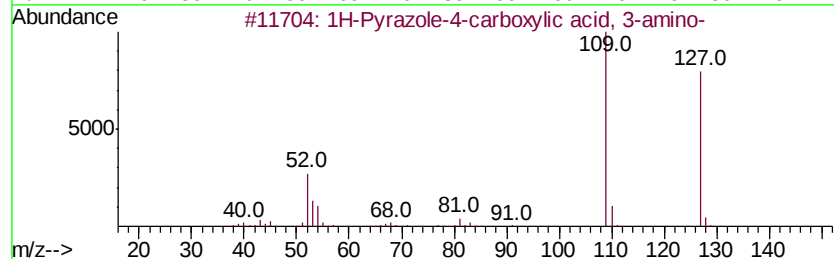
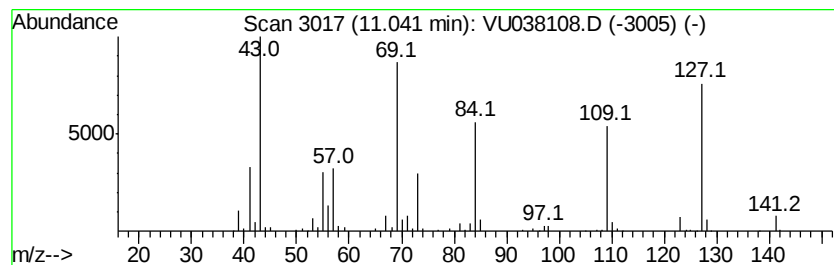
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TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.04	9.42 ug/L	409460	1,4-Dichlorobenzene-d4	11.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Pyrazole-4-carboxylic acid, 3...	127	C4H5N3O2	041680-34-6	35
2		1-Butene, 3,3-dimethyl-	84	C6H12	000558-37-2	30
3		1H-Pyrazole, 4,5-dihydro-5-methyl-	84	C4H8N2	001568-20-3	27
4		Pentane, 2-chloro-4-methyl-	120	C6H13Cl	025346-32-1	27
5		2-Pentene, 4-methyl-, (Z)-	84	C6H12	000691-38-3	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Hexanol, 2,5-di...	10.27	6.0	ug/L	263756	2	9.44	2210360	50.0
unknown-01	11.04	9.4	ug/L	409460	3	11.82	2173830	50.0