

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051022\
 Data File : VU048493.D
 Acq On : 10 May 2022 16:00
 Operator : SY/MD
 Sample : N2736-14
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXEX0

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
 Title : VOC Analysis

Signal : TIC: VU048493.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	74	81	93	rBV	129374	143274	13.06%	1.560%
2	1.912	171	178	194	rVB	95332	125152	11.41%	1.362%
3	1.996	198	204	213	rVB	21217	28822	2.63%	0.314%
4	2.568	370	382	396	rBV	230109	372867	34.00%	4.059%
5	2.761	438	442	445	rBV2	503	424	0.04%	0.005%
6	2.980	507	510	513	rBV2	483	369	0.03%	0.004%
7	3.173	550	570	586	rVB4	21311	66426	6.06%	0.723%
8	3.453	655	657	661	rVB2	310	168	0.02%	0.002%
9	3.562	687	691	692	rBV	204	151	0.01%	0.002%
10	3.578	693	696	699	rVV2	204	165	0.02%	0.002%
11	3.623	708	710	713	rBV	179	104	0.01%	0.001%
12	3.678	724	727	729	rBV	304	206	0.02%	0.002%
13	3.790	760	762	764	rBB	194	99	0.01%	0.001%
14	3.809	766	768	772	rBV2	166	111	0.01%	0.001%
15	3.851	778	781	783	rBV2	240	169	0.02%	0.002%
16	3.932	804	806	808	rBV2	156	105	0.01%	0.001%
17	4.105	858	860	864	rVB	502	268	0.02%	0.003%
18	4.160	870	877	878	rBV2	813	807	0.07%	0.009%
19	4.224	896	897	898	rBV	205	68	0.01%	0.001%
20	4.362	937	940	942	rBV2	449	311	0.03%	0.003%
21	4.430	955	961	964	rBV4	1215	1369	0.12%	0.015%
22	4.620	1007	1020	1044	rBV	130768	313379	28.57%	3.412%
23	4.941	1118	1120	1121	rBV	299	120	0.01%	0.001%
24	5.063	1142	1158	1178	rBV2	206358	451800	41.19%	4.919%
25	5.269	1220	1222	1225	rVB	218	102	0.01%	0.001%
26	5.285	1225	1227	1229	rBV	567	323	0.03%	0.004%
27	5.321	1236	1238	1241	rBV2	317	168	0.02%	0.002%
28	5.391	1246	1260	1272	rBV6	17095	37502	3.42%	0.408%
29	5.465	1273	1283	1293	rVB8	4410	9416	0.86%	0.103%
30	5.517	1297	1299	1305	rVB2	305	274	0.02%	0.003%
31	5.552	1306	1310	1318	rBV	410	517	0.05%	0.006%
32	5.591	1320	1322	1327	rBV2	190	116	0.01%	0.001%
33	5.639	1327	1337	1344	rBV4	4751	8802	0.80%	0.096%
34	5.726	1344	1364	1375	rBV2	402078	1096804	100.00%	11.941%
35	5.954	1431	1435	1436	rBV3	735	493	0.04%	0.005%
36	6.070	1468	1471	1474	rVB2	387	282	0.03%	0.003%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
 Title : VOC Analysis

37	6.105	1474	1482	1483	rBV	578	523	0.05%	0.006%
38	6.131	1489	1490	1491	rBV	247	64	0.01%	0.001%
39	6.250	1513	1527	1544	rBV	347817	652966	59.53%	7.109%
40	6.417	1576	1579	1586	rVB	553	581	0.05%	0.006%
41	6.459	1586	1592	1594	rBV3	280	345	0.03%	0.004%
42	6.530	1603	1614	1616	rBV4	2068	2785	0.25%	0.030%
43	6.690	1649	1664	1695	rBV	249657	498207	45.42%	5.424%
44	6.851	1709	1714	1717	rBV4	581	577	0.05%	0.006%
45	6.893	1724	1727	1730	rBV	308	264	0.02%	0.003%
46	6.986	1752	1756	1757	rBV2	245	163	0.01%	0.002%
47	6.999	1757	1760	1761	rBV2	794	507	0.05%	0.006%
48	7.054	1774	1777	1778	rBV2	158	70	0.01%	0.001%
49	7.169	1801	1813	1815	rBV4	5791	9655	0.88%	0.105%
50	7.227	1829	1831	1834	rBV	312	236	0.02%	0.003%
51	7.276	1842	1846	1847	rBV	239	159	0.01%	0.002%
52	7.314	1855	1858	1860	rBV2	253	153	0.01%	0.002%
53	7.401	1872	1885	1890	rBV5	2469	4387	0.40%	0.048%
54	7.485	1909	1911	1913	rBV3	325	132	0.01%	0.001%
55	7.494	1913	1914	1919	rVB	367	207	0.02%	0.002%
56	7.513	1919	1920	1923	rBV	204	76	0.01%	0.001%
57	7.565	1923	1936	1965	rBV	104638	206692	18.84%	2.250%
58	7.690	1967	1975	1984	rVB9	4213	7522	0.69%	0.082%
59	7.758	1990	1996	2000	rBV5	1173	1431	0.13%	0.016%
60	7.899	2021	2040	2055	rBV	497373	864510	78.82%	9.412%
61	8.041	2076	2084	2093	rVB7	4461	7528	0.69%	0.082%
62	8.179	2115	2127	2142	rBV3	74124	128178	11.69%	1.395%
63	8.452	2209	2212	2213	rBV2	405	242	0.02%	0.003%
64	8.488	2213	2223	2235	rVB3	9404	17034	1.55%	0.185%
65	8.536	2235	2238	2240	rBV2	326	192	0.02%	0.002%
66	8.575	2241	2250	2257	rBV	12156	19052	1.74%	0.207%
67	8.632	2257	2268	2287	rBV	409988	719483	65.60%	7.833%
68	8.877	2342	2344	2346	rBV	430	200	0.02%	0.002%
69	8.893	2348	2349	2351	rVV2	453	162	0.01%	0.002%
70	9.198	2438	2444	2453	rVB6	5528	7956	0.73%	0.087%
71	9.269	2459	2466	2476	rVB4	6621	10370	0.95%	0.113%
72	9.330	2477	2485	2497	rVB7	7094	11677	1.06%	0.127%
73	9.417	2500	2512	2536	rBV	503364	846428	77.17%	9.215%
74	9.693	2590	2598	2607	rVB7	3272	4644	0.42%	0.051%
75	9.819	2635	2637	2641	rBV2	293	203	0.02%	0.002%
76	9.880	2649	2656	2661	rBV5	2205	2915	0.27%	0.032%

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Min Area: 0 % of largest Peak

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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77	10.057	2710	2711	2713	rBV5	253	115	0.01%	0.001%
78	10.163	2741	2744	2746	rBV	359	231	0.02%	0.003%
79	10.301	2784	2787	2788	rBV	373	190	0.02%	0.002%
80	10.362	2793	2806	2826	rVV2	73769	134853	12.30%	1.468%
81	10.481	2838	2843	2854	rVB5	11836	19166	1.75%	0.209%
82	10.542	2856	2862	2870	rVV8	4502	7233	0.66%	0.079%
83	10.648	2884	2895	2903	rBV10	6288	11676	1.06%	0.127%
84	10.755	2917	2928	2950	rVB	378076	611970	55.80%	6.662%
85	11.063	3020	3024	3031	rVB8	4164	4796	0.44%	0.052%
86	11.272	3086	3089	3090	rBV2	588	321	0.03%	0.003%
87	11.523	3163	3167	3170	rBV4	1023	910	0.08%	0.010%
88	11.594	3187	3189	3190	rBV4	351	120	0.01%	0.001%
89	11.607	3190	3193	3197	rBV3	643	555	0.05%	0.006%
90	11.748	3228	3237	3244	rBV6	2750	4931	0.45%	0.054%
91	11.812	3244	3257	3274	rBV	541475	855172	77.97%	9.310%
92	11.999	3312	3315	3316	rBV3	1266	723	0.07%	0.008%
93	12.192	3363	3375	3394	rVB	517850	836225	76.24%	9.104%
94	13.005	3626	3628	3632	rVB2	747	448	0.04%	0.005%
95	13.449	3759	3766	3774	rVB5	1875	2591	0.24%	0.028%
96	13.594	3805	3811	3816	rBV5	1060	1295	0.12%	0.014%
97	13.658	3828	3831	3833	rBV2	447	304	0.03%	0.003%
98	13.819	3879	3881	3884	rBV	246	148	0.01%	0.002%
99	14.330	4036	4040	4049	rBV2	904	1107	0.10%	0.012%
100	15.500	4402	4404	4406	rBV3	1015	396	0.04%	0.004%

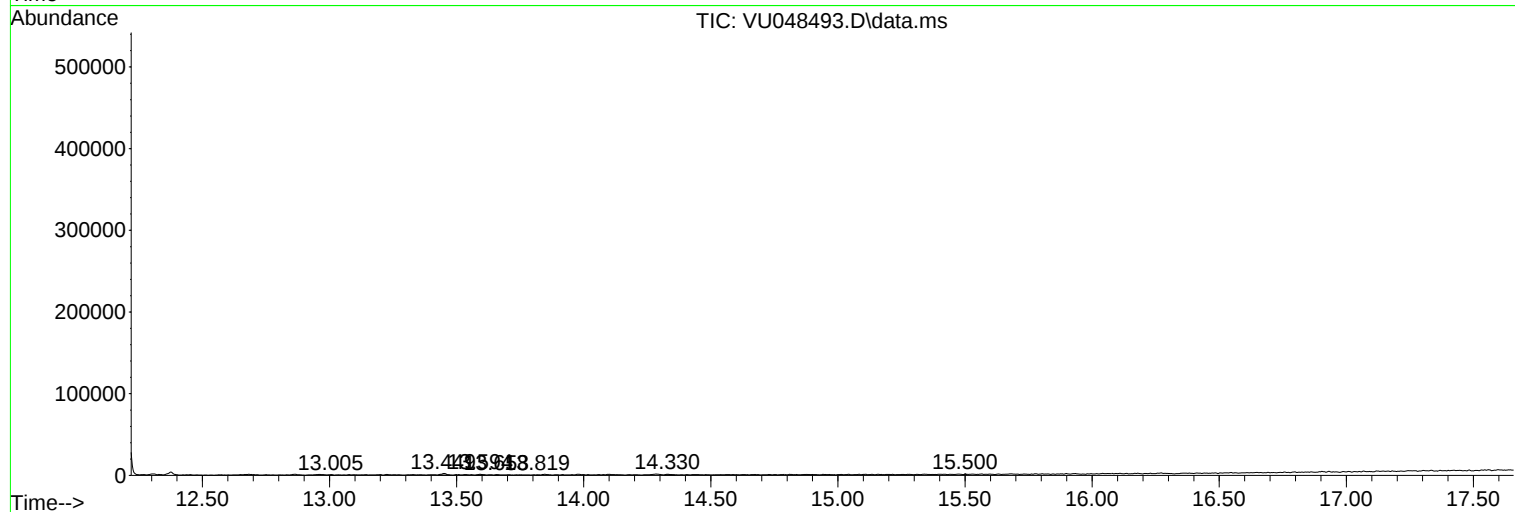
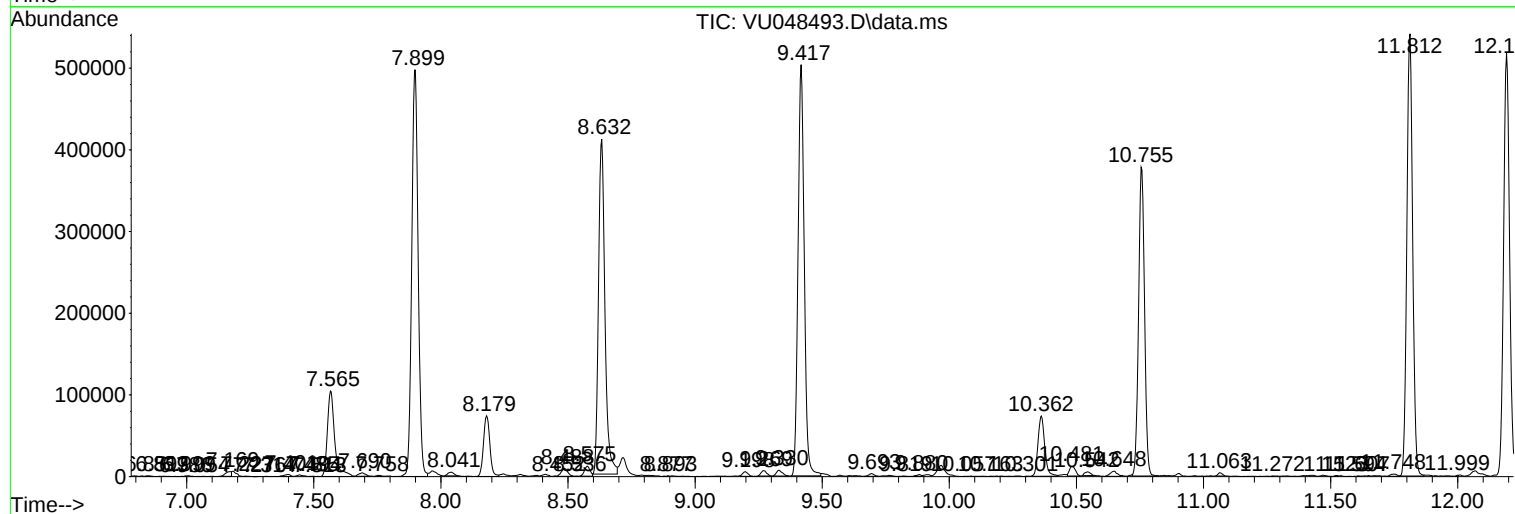
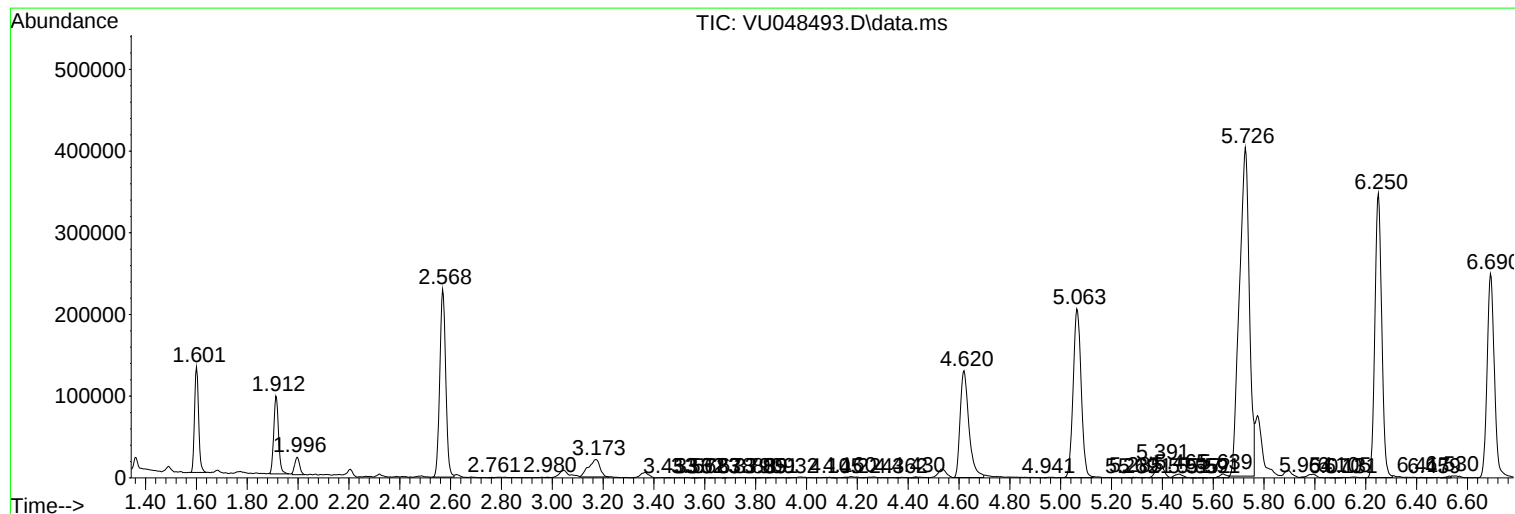
Sum of corrected areas: 9185485

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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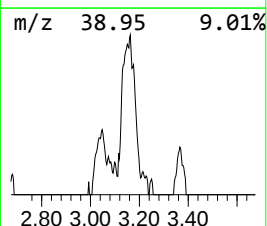
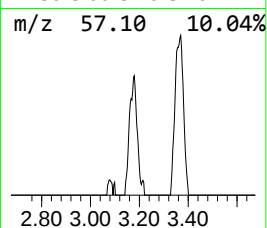
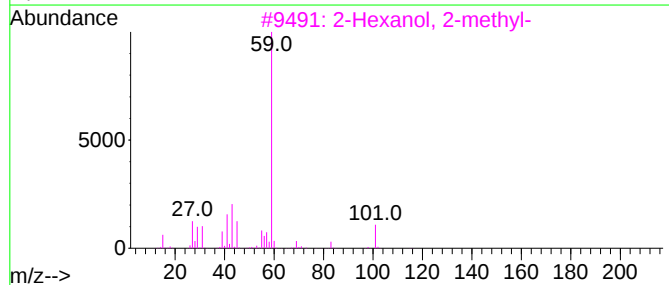
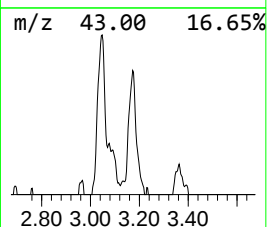
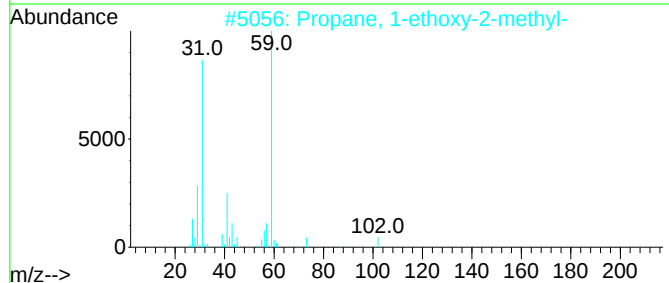
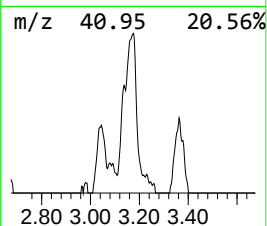
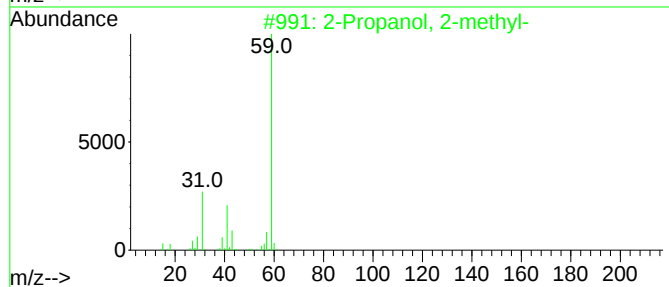
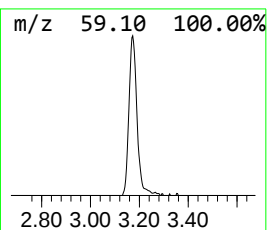
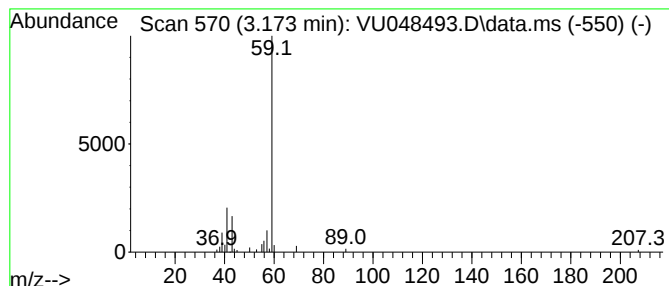
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Propanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.173	5.09 ug/L	66426	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-			74	C4H10O	000075-65-0	64
2	Propane, 1-ethoxy-2-methyl-			102	C6H14O	000627-02-1	43
3	2-Hexanol, 2-methyl-			116	C7H16O	000625-23-0	40
4	3-Pentanol			88	C5H12O	000584-02-1	40
5	3-Hydroxy-3-methyl-2-butanone			102	C5H10O2	000115-22-0	39



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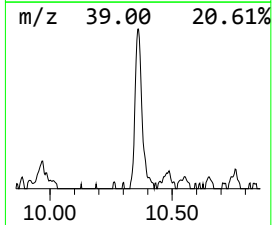
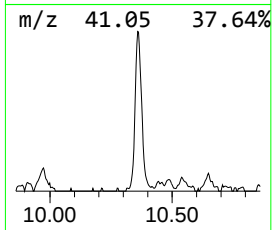
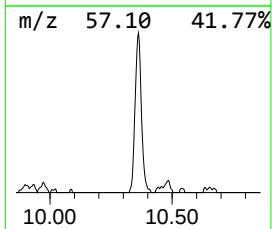
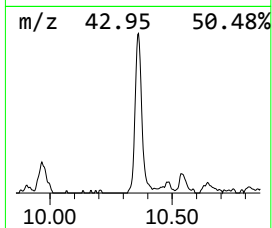
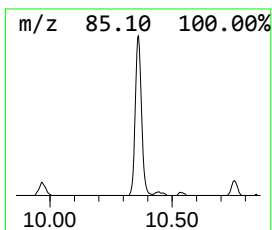
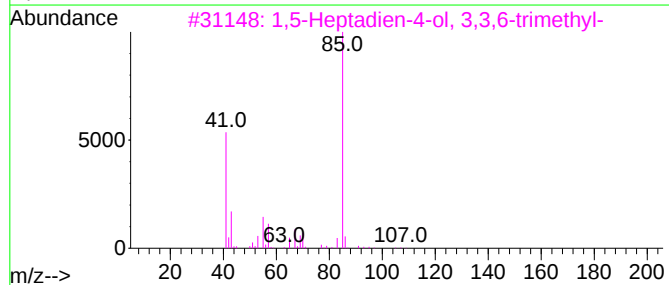
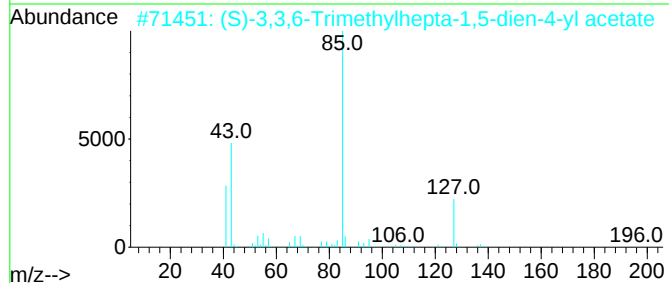
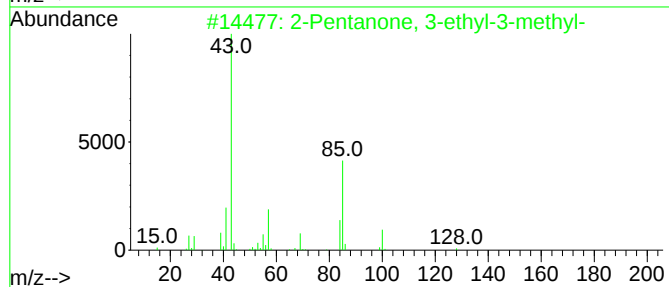
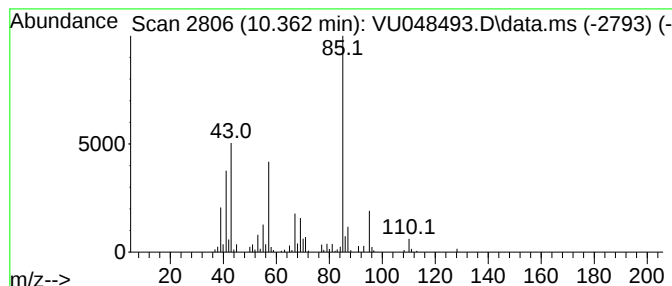
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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 3-ethyl-3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.362	7.97 ug/L	134853	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 3-ethyl-3-methyl-	128	C8H16O	019780-65-5	58
2			(S)-3,3,6-Trimethylhepta-1,5-die...	196	C12H20O2	003465-88-1	53
3			1,5-Heptadien-4-ol, 3,3,6-trimet...	154	C10H18O	027644-04-8	53
4			Pentane, 3-ethyl-3-methyl-	114	C8H18	001067-08-9	53
5			Pentane, 3-ethyl-3-methyl-	114	C8H18	001067-08-9	50



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Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Propanol, 2-m...	3.173	5.1	ug/L	66426	1	6.250	652966	50.0
2-Pentanone, 3-...	10.362	8.0	ug/L	134853	2	9.417	846428	50.0