

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV020222\
 Data File : VV024525.D
 Acq On : 02 Feb 2022 15:24
 Operator : SY/MD
 Sample : N1353-03ME
 Misc : 3.33g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 COVE4ME

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_V\Method\SFAMVLM020222WMA.M
 Title : VOC Analysis

Signal : TIC: VV024525.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.304	76	82	97	rVB	162258	187867	13.66%	1.976%
2	1.568	157	164	178	rBV	137844	189765	13.80%	1.996%
3	2.085	316	325	337	rVB	348566	493811	35.91%	5.195%
4	3.050	622	625	629	rBV3	880	686	0.05%	0.007%
5	3.455	746	751	756	rBV8	838	769	0.06%	0.008%
6	3.542	776	778	780	rVB3	476	212	0.02%	0.002%
7	3.561	780	784	786	rBV3	752	566	0.04%	0.006%
8	3.587	790	792	795	rBV4	660	445	0.03%	0.005%
9	3.625	800	804	805	rBV3	691	394	0.03%	0.004%
10	3.751	841	843	844	rBV	281	118	0.01%	0.001%
11	3.793	853	856	858	rBV4	563	324	0.02%	0.003%
12	3.854	872	875	877	rBV3	451	264	0.02%	0.003%
13	3.902	880	890	923	rBV	61244	246217	17.91%	2.590%
14	4.346	1013	1028	1058	rVB	201857	534521	38.87%	5.623%
15	4.912	1200	1204	1208	rBV5	485	492	0.04%	0.005%
16	5.040	1226	1244	1273	rBV2	553667	1374992	100.00%	14.465%
17	5.532	1395	1397	1401	rVB3	692	401	0.03%	0.004%
18	5.612	1408	1422	1464	rBV	439286	932563	67.82%	9.811%
19	5.902	1501	1512	1531	rBV2	27468	62984	4.58%	0.663%
20	6.066	1551	1563	1581	rBV	293975	637048	46.33%	6.702%
21	6.985	1838	1849	1873	rBV	175535	353380	25.70%	3.718%
22	7.149	1898	1900	1904	rBV3	526	401	0.03%	0.004%
23	7.233	1916	1926	1935	rBV	116784	255917	18.61%	2.692%
24	7.622	2037	2047	2074	rBV	110818	236989	17.24%	2.493%
25	8.046	2176	2179	2180	rBV2	664	348	0.03%	0.004%
26	8.095	2185	2194	2197	rBV	108237	155082	11.28%	1.632%
27	8.429	2295	2298	2305	rBV5	878	958	0.07%	0.010%
28	8.490	2315	2317	2318	rBV	578	269	0.02%	0.003%
29	8.558	2335	2338	2340	rBV3	362	199	0.01%	0.002%
30	8.571	2340	2342	2344	rBV2	492	232	0.02%	0.002%
31	8.648	2364	2366	2370	rBV3	402	276	0.02%	0.003%
32	8.796	2408	2412	2416	rVB3	741	479	0.03%	0.005%
33	8.853	2416	2430	2461	rBV	560418	1128624	82.08%	11.873%
34	9.146	2513	2521	2534	rVB3	12652	24964	1.82%	0.263%
35	9.297	2566	2568	2571	rVB4	540	204	0.01%	0.002%
36	9.397	2597	2599	2603	rBV4	607	516	0.04%	0.005%

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 Title : VOC Analysis

37	9.419	2603	2606	2607	rVV3	451	228	0.02%	0.002%
38	9.461	2617	2619	2620	rBV2	562	165	0.01%	0.002%
39	9.554	2640	2648	2660	rBV3	6498	11269	0.82%	0.119%
40	9.722	2689	2700	2719	rBV	40971	83331	6.06%	0.877%
41	9.870	2740	2746	2761	rVB3	7476	12760	0.93%	0.134%
42	10.223	2843	2856	2873	rBV	301088	556198	40.45%	5.851%
43	10.660	2988	2992	2993	rBV2	678	469	0.03%	0.005%
44	10.670	2993	2995	2999	rVB2	1000	426	0.03%	0.004%
45	10.750	3015	3020	3026	rBV6	883	1284	0.09%	0.014%
46	11.030	3103	3107	3109	rBV3	1251	1120	0.08%	0.012%
47	11.149	3138	3144	3154	rVB8	2773	4600	0.33%	0.048%
48	11.252	3164	3176	3193	rBV	658698	1042376	75.81%	10.966%
49	11.538	3258	3265	3270	rBV7	2243	3614	0.26%	0.038%
50	11.628	3280	3293	3313	rBV	595039	949151	69.03%	9.985%
51	12.326	3507	3510	3512	rBV2	464	291	0.02%	0.003%
52	12.403	3530	3534	3539	rBV5	929	1147	0.08%	0.012%
53	12.461	3548	3552	3554	rBV3	877	701	0.05%	0.007%
54	12.654	3608	3612	3617	rVB6	906	1008	0.07%	0.011%
55	12.676	3617	3619	3622	rBV3	418	282	0.02%	0.003%
56	12.766	3643	3647	3650	rBV5	581	458	0.03%	0.005%
57	12.844	3668	3671	3674	rBV2	652	548	0.04%	0.006%
58	12.866	3674	3678	3679	rBV3	662	380	0.03%	0.004%
59	12.959	3705	3707	3710	rBV4	571	329	0.02%	0.003%
60	13.008	3720	3722	3726	rBV3	410	274	0.02%	0.003%
61	13.030	3726	3729	3730	rBV2	254	122	0.01%	0.001%
62	13.168	3769	3772	3773	rBV	256	131	0.01%	0.001%
63	13.229	3787	3791	3792	rBV	405	312	0.02%	0.003%
64	13.258	3798	3800	3801	rBV2	498	185	0.01%	0.002%
65	13.326	3815	3821	3824	rBV4	525	626	0.05%	0.007%
66	13.606	3904	3908	3913	rBV6	445	431	0.03%	0.005%
67	13.718	3939	3943	3945	rVB4	508	344	0.03%	0.004%
68	13.750	3945	3953	3956	rBV8	948	1065	0.08%	0.011%
69	13.766	3956	3958	3960	rBV2	365	176	0.01%	0.002%
70	13.837	3978	3980	3981	rBV	414	194	0.01%	0.002%
71	13.876	3990	3992	3994	rBV3	555	234	0.02%	0.002%
72	13.898	3997	3999	4002	rVB2	543	236	0.02%	0.002%
73	13.975	4022	4023	4026	rVB3	251	120	0.01%	0.001%
74	13.995	4026	4029	4033	rVB2	419	289	0.02%	0.003%
75	14.040	4039	4043	4044	rBV4	1007	670	0.05%	0.007%
76	14.082	4055	4056	4058	rVB	510	122	0.01%	0.001%

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 ClientSampleId :
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Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

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Stop Thrs : 0

Peak Location: TOP

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

Peak separation: 5

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Title : VOC Analysis

77	14.094	4058	4060	4061	rBV	409	206	0.01%	0.002%
78	14.143	4073	4075	4077	rBV3	454	268	0.02%	0.003%
79	14.197	4090	4092	4094	rBV4	534	257	0.02%	0.003%
80	14.236	4102	4104	4106	rBV2	494	243	0.02%	0.003%
81	14.358	4139	4142	4144	rBV3	615	436	0.03%	0.005%
82	14.725	4251	4256	4259	rBV7	656	704	0.05%	0.007%
83	14.834	4288	4290	4292	rBV2	720	314	0.02%	0.003%
84	14.882	4297	4305	4310	rBV5	1122	2111	0.15%	0.022%

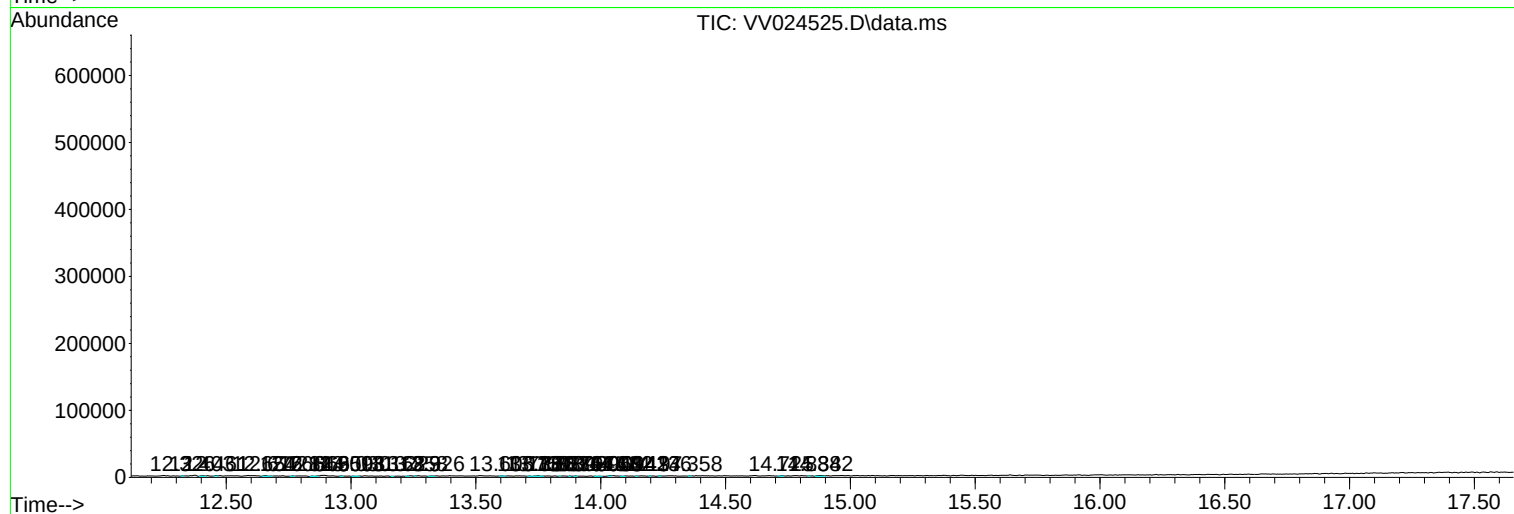
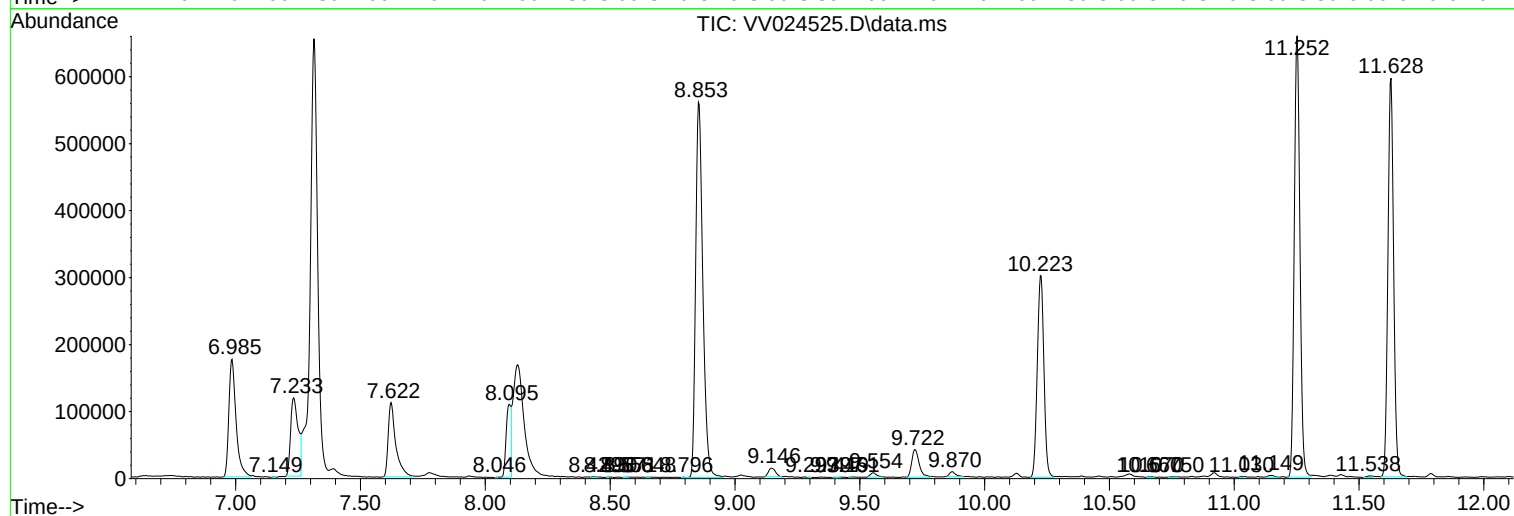
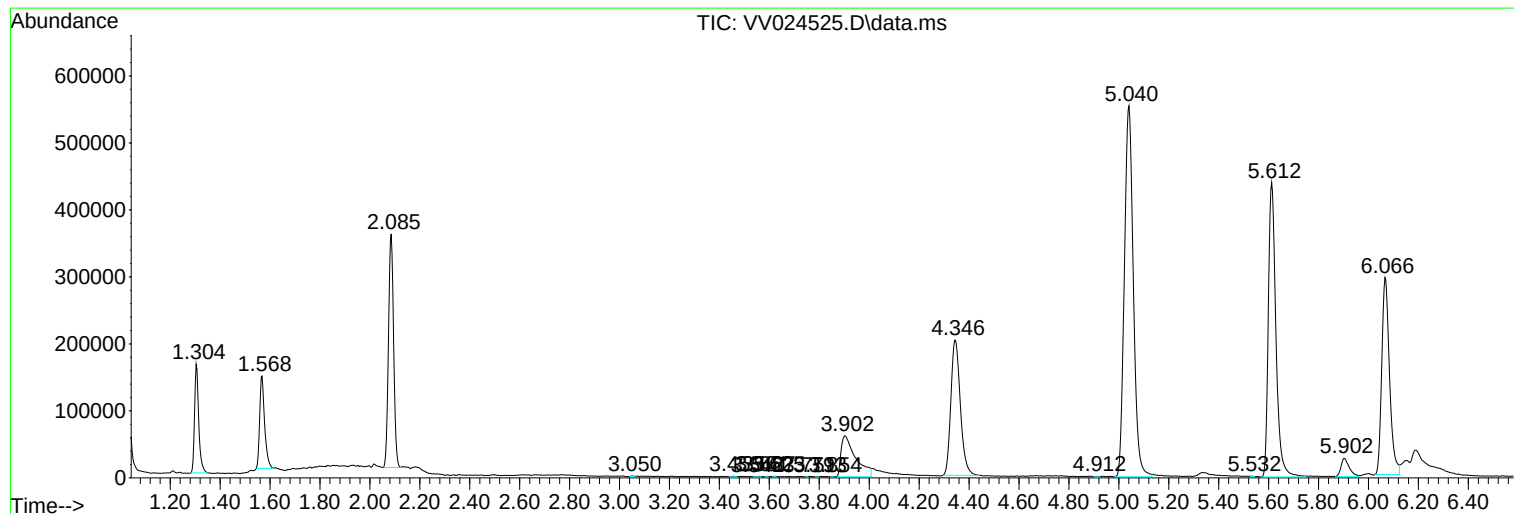
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Instrument :
MSVOA_V
ClientSampleId :
C0VE4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM020222WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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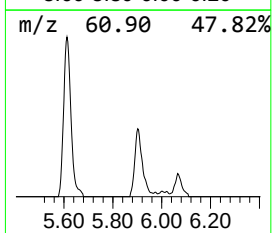
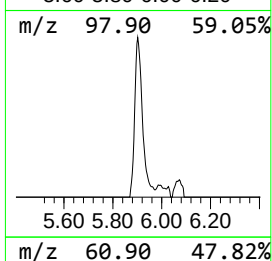
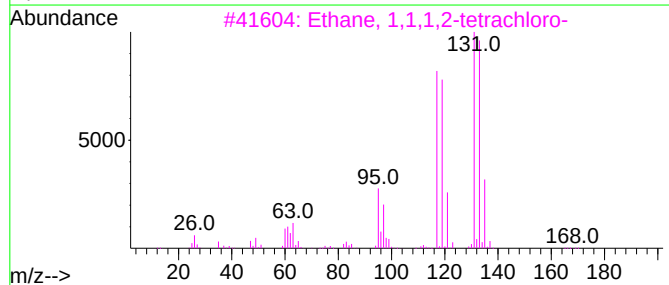
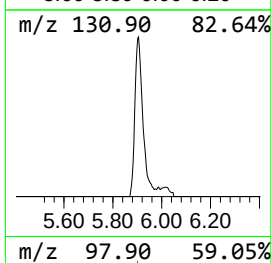
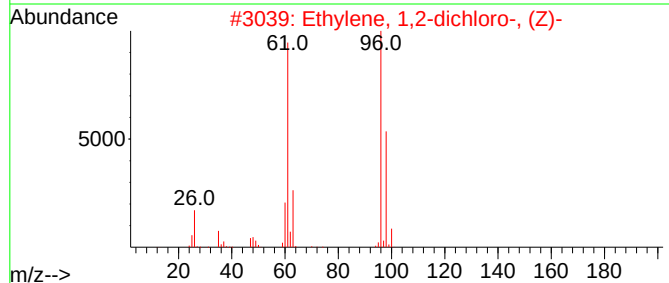
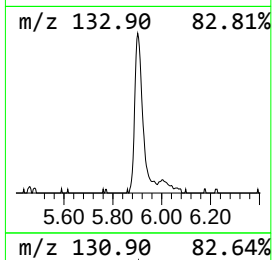
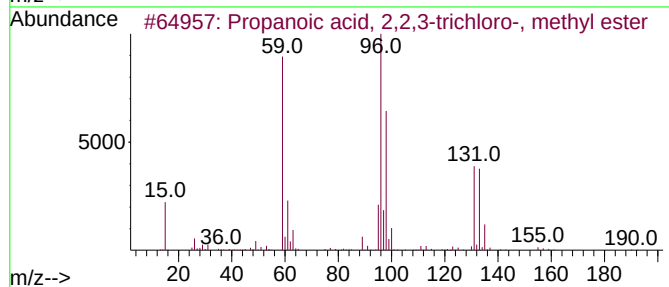
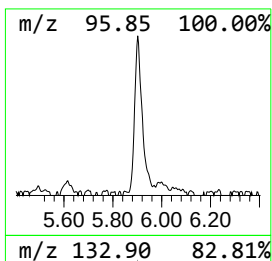
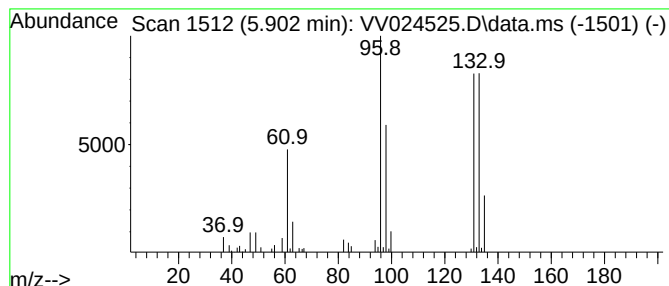
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM020222WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Propanoic acid, 2,2,3-trich... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.902	3.38 ug/L	62984	1,4-Difluorobenzene	5.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	50
2			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	35
3			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	23
4			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	10
5			4(1H)-Pyrimidinone	96	C4H4N2O	004562-27-0	9



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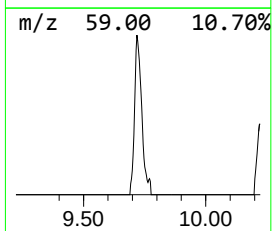
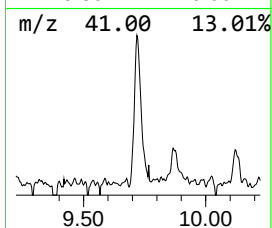
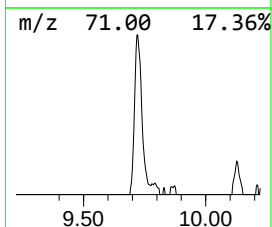
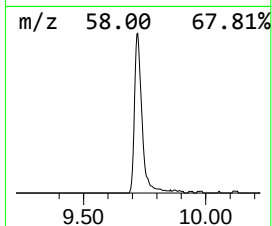
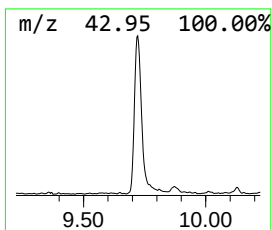
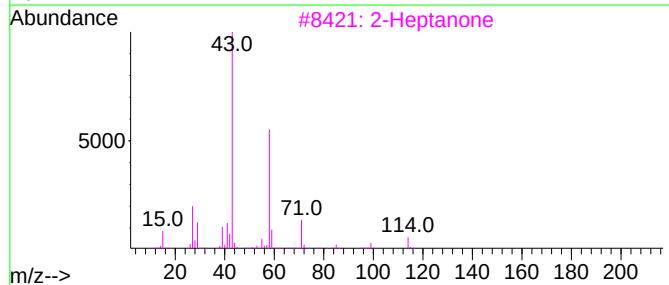
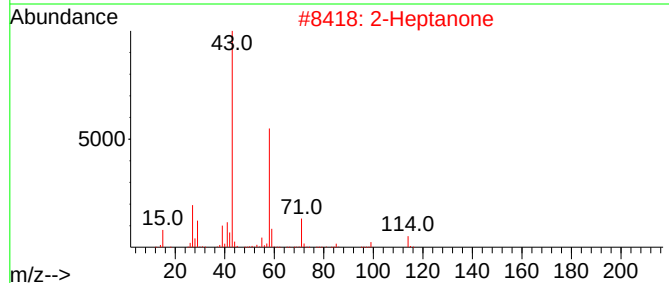
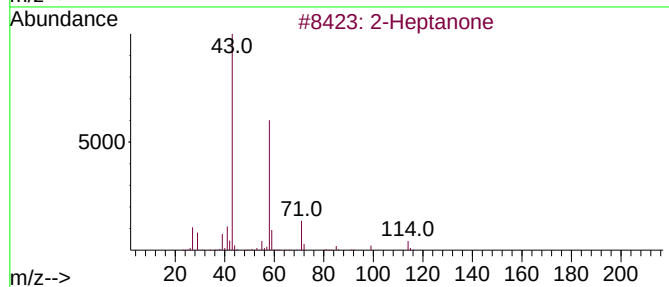
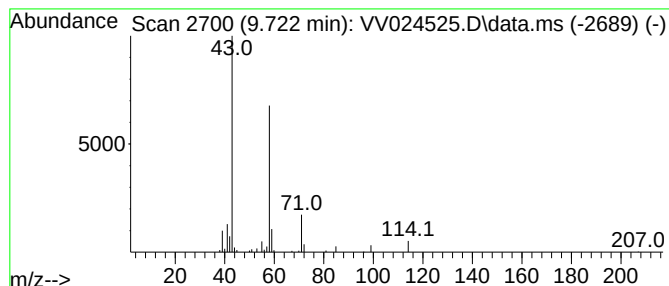
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Quant Title : VOC Analysis

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

Peak Number 3 2-Heptanone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.722	3.69 ug/L	83331	Chlorobenzene-d5	8.853

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Heptanone			114	C7H14O	000110-43-0	91
2	2-Heptanone			114	C7H14O	000110-43-0	91
3	2-Heptanone			114	C7H14O	000110-43-0	91
4	2-Heptanone			114	C7H14O	000110-43-0	90
5	2-Hexanone, 5-methyl-			114	C7H14O	000110-12-3	86



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.902	3.4	ug/L	62984	1	5.612	932563	50.0
2-Heptanone	9.722	3.7	ug/L	83331	2	8.853	1128620	50.0