

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV061523\
 Data File : VV031525.D
 Acq On : 15 Jun 2023 12:55
 Operator : SY/MD
 Sample : 03249-01
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 EXYS3

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\SFAMVLM061423WMA.M
 Title : VOC Analysis

Signal : TIC: VV031525.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.176	37	42	51	rBV	15738	17886	0.96%	0.181%
2	1.285	69	76	95	rVB2	316977	346914	18.67%	3.510%
3	1.555	149	160	171	rVB2	232140	340553	18.33%	3.446%
4	2.066	310	319	337	rVB2	148468	223579	12.04%	2.262%
5	2.455	433	440	448	rBV5	1732	2831	0.15%	0.029%
6	2.593	471	483	495	rBV4	2634	6065	0.33%	0.061%
7	2.703	507	517	535	rBV	30515	54217	2.92%	0.549%
8	2.790	542	544	545	rBV2	224	103	0.01%	0.001%
9	2.825	552	555	557	rVB	318	144	0.01%	0.001%
10	2.851	561	563	566	rVV2	250	149	0.01%	0.002%
11	2.870	566	569	575	rVB2	223	189	0.01%	0.002%
12	2.921	580	585	589	rBV2	279	275	0.01%	0.003%
13	3.121	631	647	674	rBV	829312	1737504	93.53%	17.579%
14	3.507	763	767	771	rBV	591	549	0.03%	0.006%
15	3.629	801	805	809	rBV2	293	286	0.02%	0.003%
16	3.648	809	811	816	rVV2	209	168	0.01%	0.002%
17	3.674	816	819	821	rVB3	245	136	0.01%	0.001%
18	3.693	821	825	826	rBV	230	108	0.01%	0.001%
19	3.725	832	835	838	rBV	234	133	0.01%	0.001%
20	3.741	838	840	844	rBV2	198	156	0.01%	0.002%
21	3.822	848	865	906	rBV2	725393	1857735	100.00%	18.796%
22	4.259	988	1001	1026	rVB	108236	274375	14.77%	2.776%
23	4.523	1064	1083	1112	rBV	260110	676677	36.42%	6.846%
24	4.735	1146	1149	1151	rBV2	529	429	0.02%	0.004%
25	4.802	1165	1170	1172	rBV2	254	238	0.01%	0.002%
26	4.880	1191	1194	1196	rBV2	393	225	0.01%	0.002%
27	4.966	1203	1221	1241	rBV2	238948	646206	34.78%	6.538%
28	5.246	1305	1308	1310	rBV2	405	264	0.01%	0.003%
29	5.291	1320	1322	1325	rBV	234	101	0.01%	0.001%
30	5.310	1325	1328	1330	rBV2	252	158	0.01%	0.002%
31	5.458	1370	1374	1376	rBV2	225	210	0.01%	0.002%
32	5.542	1389	1400	1423	rBV2	178805	370580	19.95%	3.749%
33	5.741	1459	1462	1465	rBV2	274	207	0.01%	0.002%
34	5.844	1481	1494	1515	rBV3	35087	74829	4.03%	0.757%
35	5.934	1520	1522	1526	rBV4	602	423	0.02%	0.004%
36	5.995	1529	1541	1567	rBV2	146736	309363	16.65%	3.130%

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 Title : VOC Analysis

37	6.230	1611	1614	1619	rVB2	157	156	0.01%	0.002%
38	6.333	1638	1646	1651	rBV5	2328	3736	0.20%	0.038%
39	6.442	1677	1680	1685	rBV3	368	294	0.02%	0.003%
40	6.526	1703	1706	1708	rBV	228	143	0.01%	0.001%
41	6.587	1723	1725	1726	rBV2	299	141	0.01%	0.001%
42	6.728	1761	1769	1773	rBV2	353	504	0.03%	0.005%
43	6.921	1811	1829	1846	rBV	72326	135854	7.31%	1.375%
44	7.140	1892	1897	1900	rBV5	615	550	0.03%	0.006%
45	7.249	1918	1931	1949	rBV	242187	431733	23.24%	4.368%
46	7.561	2018	2028	2052	rBV3	54071	99296	5.35%	1.005%
47	7.783	2088	2097	2109	rVV6	1535	3035	0.16%	0.031%
48	7.838	2111	2114	2115	rVV2	402	208	0.01%	0.002%
49	7.847	2115	2117	2119	rVV2	516	289	0.02%	0.003%
50	7.912	2120	2137	2156	rVB3	27059	53959	2.90%	0.546%
51	8.034	2165	2175	2213	rBV	184703	346310	18.64%	3.504%
52	8.394	2284	2287	2289	rBV2	381	297	0.02%	0.003%
53	8.471	2308	2311	2312	rBV2	256	138	0.01%	0.001%
54	8.584	2344	2346	2348	rBV2	208	105	0.01%	0.001%
55	8.619	2354	2357	2360	rBV2	220	158	0.01%	0.002%
56	8.641	2360	2364	2366	rVV	315	215	0.01%	0.002%
57	8.793	2397	2411	2433	rBV	275457	458438	24.68%	4.638%
58	9.063	2493	2495	2497	rVV3	283	162	0.01%	0.002%
59	9.076	2497	2499	2500	rVV	530	279	0.02%	0.003%
60	9.092	2500	2504	2515	rVV5	1521	2059	0.11%	0.021%
61	9.133	2515	2517	2519	rVB	222	107	0.01%	0.001%
62	9.362	2586	2588	2595	rVB	355	301	0.02%	0.003%
63	9.487	2623	2627	2629	rBV2	923	831	0.04%	0.008%
64	9.680	2684	2687	2689	rBV2	392	273	0.01%	0.003%
65	9.773	2712	2716	2719	rVB3	291	248	0.01%	0.003%
66	9.841	2731	2737	2740	rBV2	313	232	0.01%	0.002%
67	9.879	2740	2749	2757	rBV2	1836	2350	0.13%	0.024%
68	9.969	2775	2777	2778	rBV2	259	112	0.01%	0.001%
69	10.018	2789	2792	2798	rBV	271	260	0.01%	0.003%
70	10.101	2815	2818	2820	rBV	203	106	0.01%	0.001%
71	10.114	2820	2822	2824	rVV2	302	154	0.01%	0.002%
72	10.159	2825	2836	2859	rVB	242153	382591	20.59%	3.871%
73	10.256	2864	2866	2873	rBV2	357	344	0.02%	0.003%
74	10.391	2906	2908	2912	rBV2	267	221	0.01%	0.002%
75	10.410	2912	2914	2918	rVV2	351	219	0.01%	0.002%
76	10.429	2918	2920	2922	rVV2	216	104	0.01%	0.001%

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 Title : VOC Analysis

77	10.487	2932	2938	2945	rVB2	1326	1632	0.09%	0.017%
78	10.683	2990	2999	3011	rVB4	3242	4904	0.26%	0.050%
79	10.860	3046	3054	3063	rBV	6969	9208	0.50%	0.093%
80	11.043	3108	3111	3114	rBV3	288	194	0.01%	0.002%
81	11.130	3133	3138	3145	rVB4	963	1489	0.08%	0.015%
82	11.191	3145	3157	3177	rBV	277520	430702	23.18%	4.358%
83	11.474	3236	3245	3252	rBV4	2461	3766	0.20%	0.038%
84	11.567	3262	3274	3295	rBV	291560	453514	24.41%	4.588%
85	11.866	3357	3367	3385	rBV	58665	98858	5.32%	1.000%
86	11.989	3403	3405	3407	rBV	285	148	0.01%	0.001%
87	12.104	3439	3441	3444	rBV2	391	230	0.01%	0.002%
88	12.201	3460	3471	3482	rBV3	1992	3691	0.20%	0.037%
89	12.423	3535	3540	3544	rBV3	300	384	0.02%	0.004%
90	12.982	3711	3714	3718	rBV2	538	405	0.02%	0.004%
91	13.053	3734	3736	3737	rBV	391	170	0.01%	0.002%
92	13.111	3752	3754	3760	rVB2	592	501	0.03%	0.005%
93	13.146	3762	3765	3767	rBV	445	301	0.02%	0.003%
94	13.300	3810	3813	3814	rBV	489	291	0.02%	0.003%
95	13.526	3881	3883	3888	rBV2	357	250	0.01%	0.003%
96	13.689	3930	3934	3940	rVB3	1018	1075	0.06%	0.011%
97	13.850	3981	3984	3986	rBV	368	195	0.01%	0.002%
98	13.921	4004	4006	4014	rVB	583	573	0.03%	0.006%
99	13.960	4014	4018	4020	rBV4	566	483	0.03%	0.005%
100	14.554	4201	4203	4204	rBV	584	272	0.01%	0.003%

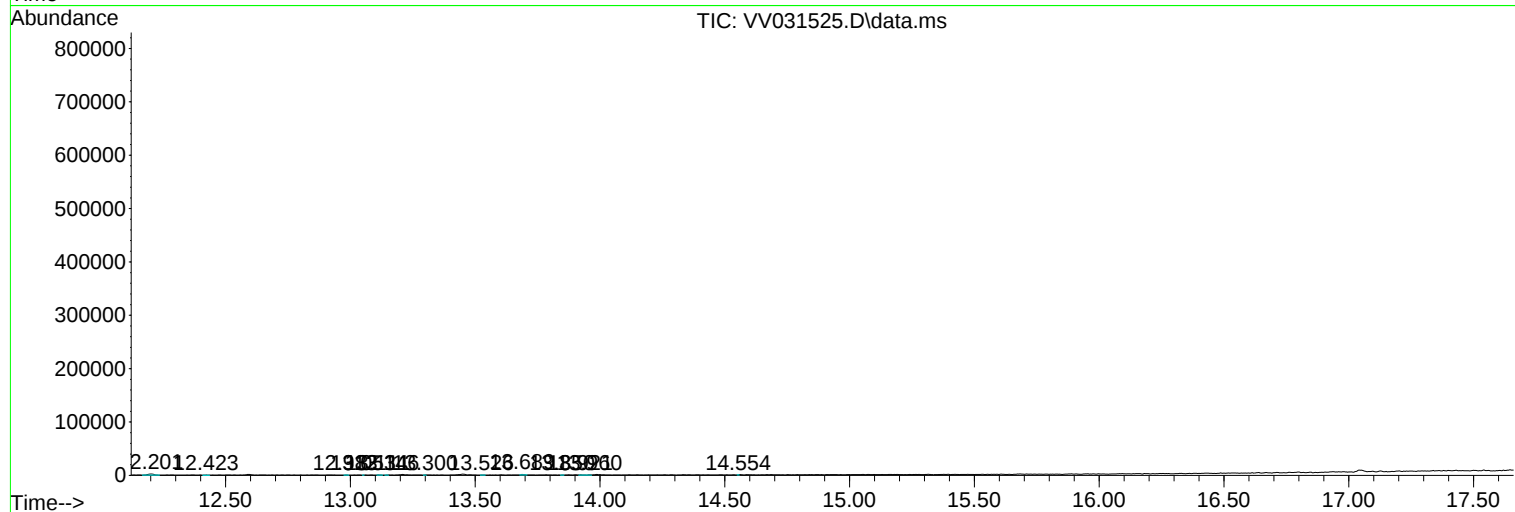
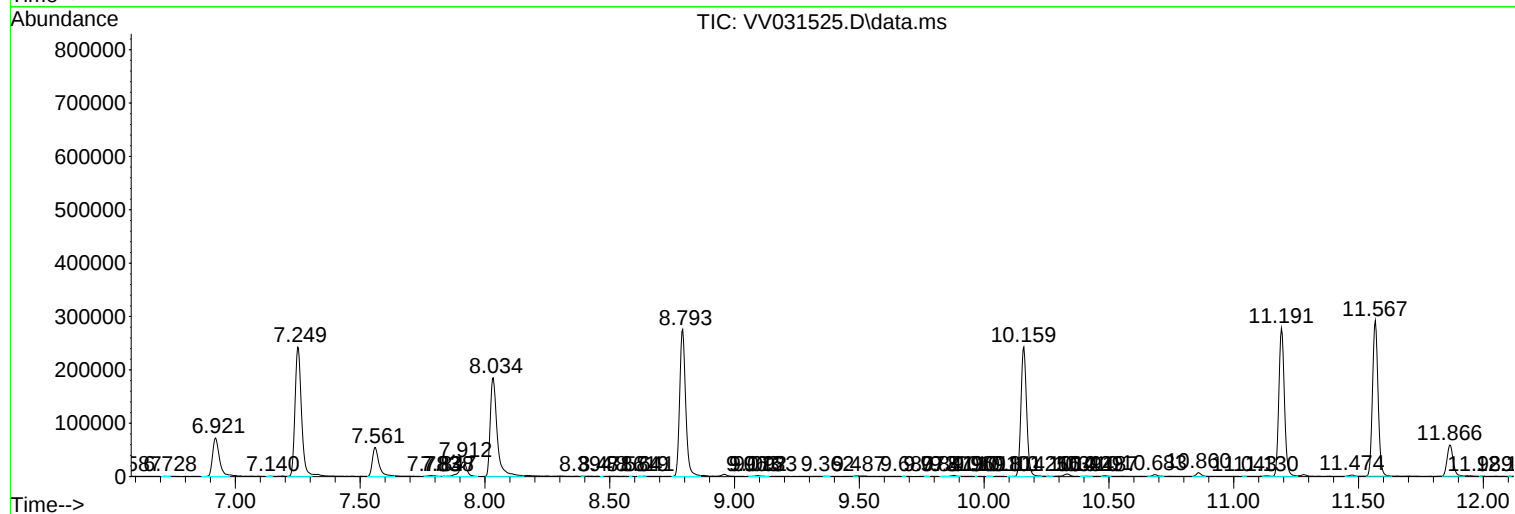
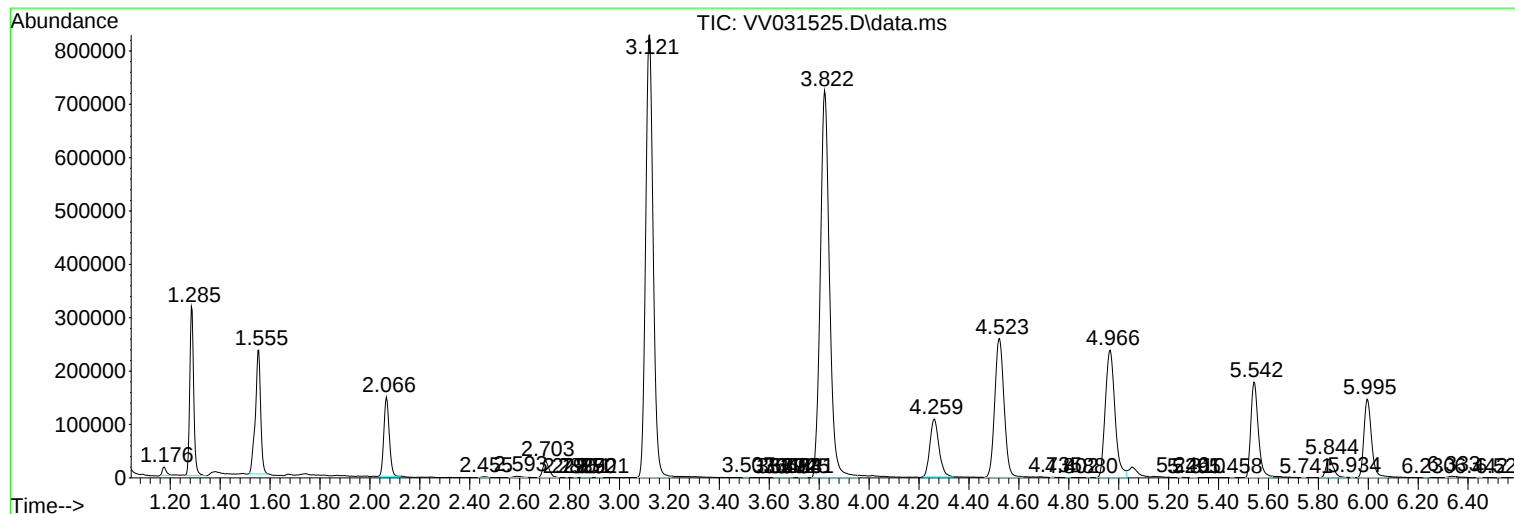
Sum of corrected areas: 9883713

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

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



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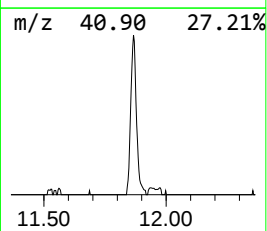
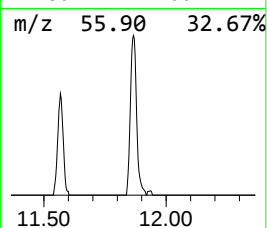
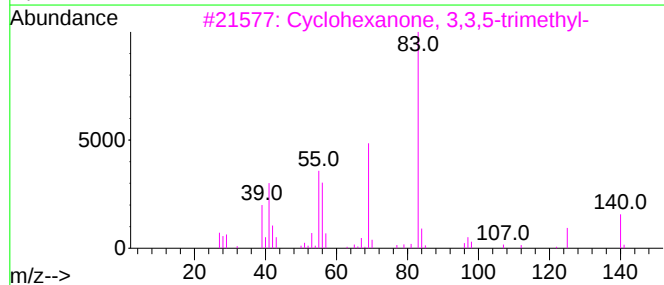
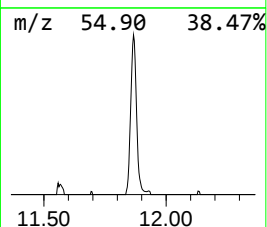
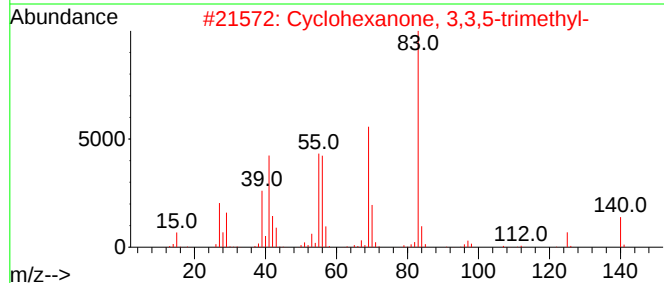
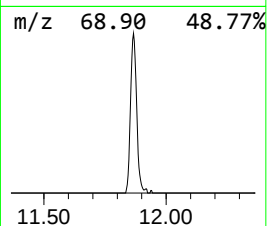
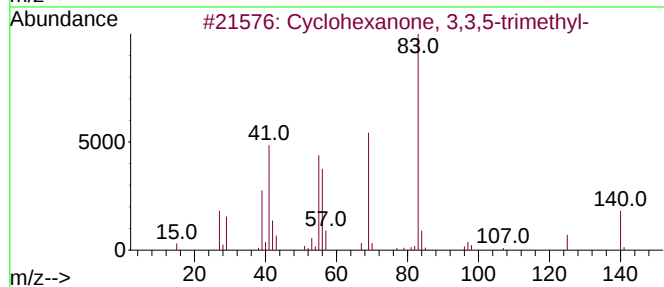
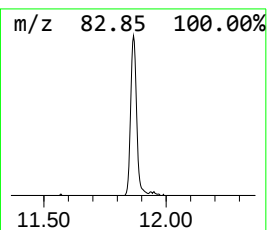
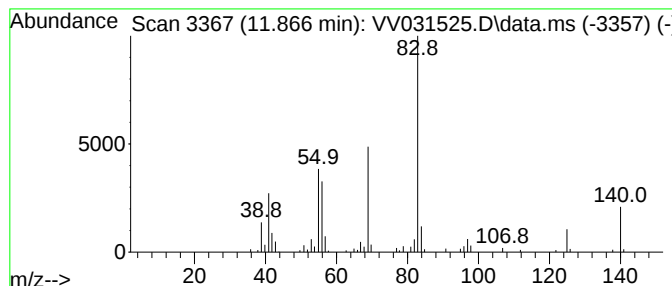
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM061423WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Cyclohexanone, 3,3,5-trimet... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.866	11.48 ug/L	98858	1,4-Dichlorobenzene-d4	11.191

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	91
2			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	91
3			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	90
4			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	70
5			Cyclopentanone, 2,4,4-trimethyl-	126	C8H14O	004694-12-6	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexanone, ...	11.866	11.5	ug/L	98858	3	11.191	430702	50.0