

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV081924\
 Data File : VV036976.D
 Acq On : 19 Aug 2024 14:34
 Operator : SY/MD
 Sample : P3593-01 10X
 Misc : 5.00mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DCXW2

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\SFAMVLM080224WMA.M
 Title : VOC Analysis

Signal : TIC: VV036976.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.220	51	56	57	rBV3	4464	4344	0.17%	0.021%
2	1.278	67	74	88	rBV	345059	367498	13.98%	1.747%
3	1.532	145	153	172	rVB	294668	362040	13.77%	1.721%
4	2.060	307	317	326	rBV	602731	870430	33.11%	4.137%
5	2.111	326	333	359	rVB	355412	579329	22.03%	2.754%
6	2.445	429	437	452	rVB2	55259	92707	3.53%	0.441%
7	3.323	704	710	713	rBV5	2544	3044	0.12%	0.014%
8	3.355	718	720	723	rBV3	1638	940	0.04%	0.004%
9	3.548	778	780	784	rVB5	1211	821	0.03%	0.004%
10	3.693	820	825	828	rVB6	1490	1432	0.05%	0.007%
11	3.728	834	836	840	rBV6	1288	1053	0.04%	0.005%
12	3.796	848	857	881	rBV	167343	444888	16.92%	2.115%
13	4.243	979	996	1022	rBV	418430	1054407	40.10%	5.012%
14	4.362	1030	1033	1037	rBV5	1444	871	0.03%	0.004%
15	4.699	1136	1138	1141	rVB2	1553	774	0.03%	0.004%
16	4.732	1146	1148	1152	rVB4	1624	1056	0.04%	0.005%
17	4.770	1157	1160	1170	rVB4	1805	1995	0.08%	0.009%
18	4.809	1170	1172	1176	rBV4	942	809	0.03%	0.004%
19	4.896	1196	1199	1201	rBV3	1471	701	0.03%	0.003%
20	4.950	1201	1216	1241	rBV2	1052775	2629276	100.00%	12.497%
21	5.230	1301	1303	1306	rBV3	1620	726	0.03%	0.003%
22	5.387	1346	1352	1355	rBV7	1220	1370	0.05%	0.007%
23	5.436	1365	1367	1370	rBV4	1504	863	0.03%	0.004%
24	5.452	1370	1372	1374	rBV3	1338	682	0.03%	0.003%
25	5.532	1385	1397	1429	rBV	750577	1551098	58.99%	7.373%
26	5.986	1526	1538	1566	rBV	592816	1208855	45.98%	5.746%
27	6.268	1619	1626	1647	rVB	68451	134835	5.13%	0.641%
28	6.912	1814	1826	1851	rBV	336095	636423	24.21%	3.025%
29	7.169	1898	1906	1917	rBV3	25363	45659	1.74%	0.217%
30	7.239	1917	1928	1966	rVB	1208286	2130098	81.01%	10.125%
31	7.551	2015	2025	2048	rBV2	227165	409526	15.58%	1.947%
32	7.866	2116	2123	2130	rBV3	9482	15103	0.57%	0.072%
33	7.953	2142	2150	2158	rBV2	27206	48454	1.84%	0.230%
34	8.021	2160	2171	2210	rVB3	687283	1350587	51.37%	6.420%
35	8.477	2311	2313	2315	rBV3	1277	686	0.03%	0.003%
36	8.532	2328	2330	2334	rBV5	1933	1559	0.06%	0.007%

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Title : VOC Analysis

37	8.632	2353	2361	2369	rBV9	5478	8584	0.33%	0.041%
38	8.780	2396	2407	2442	rBV	1206783	1986162	75.54%	9.441%
39	9.185	2531	2533	2537	rVB5	2128	1431	0.05%	0.007%
40	9.207	2537	2540	2541	rBV3	1784	812	0.03%	0.004%
41	9.249	2551	2553	2556	rBV3	1497	735	0.03%	0.003%
42	9.291	2564	2566	2568	rBV3	1238	716	0.03%	0.003%
43	9.336	2573	2580	2597	rVB3	9357	20524	0.78%	0.098%
44	9.448	2611	2615	2619	rBV6	1309	1034	0.04%	0.005%
45	9.509	2631	2634	2637	rBV4	1350	935	0.04%	0.004%
46	9.706	2691	2695	2696	rBV3	1782	1100	0.04%	0.005%
47	9.805	2723	2726	2728	rBV4	1257	693	0.03%	0.003%
48	9.828	2730	2733	2736	rVV4	1326	1066	0.04%	0.005%
49	9.944	2766	2769	2770	rBV3	1181	719	0.03%	0.003%
50	9.953	2770	2772	2776	rVV4	1688	1390	0.05%	0.007%
51	10.149	2818	2833	2850	rVV	751106	1192536	45.36%	5.668%
52	10.320	2881	2886	2895	rVV8	3282	5113	0.19%	0.024%
53	10.403	2911	2912	2917	rVB4	1364	681	0.03%	0.003%
54	10.471	2927	2933	2937	rBV7	1749	2234	0.08%	0.011%
55	10.612	2973	2977	2981	rVB6	997	768	0.03%	0.004%
56	10.635	2981	2984	2989	rBV7	2520	2191	0.08%	0.010%
57	10.680	2995	2998	3001	rBV6	1046	833	0.03%	0.004%
58	10.696	3001	3003	3006	rVV4	1751	1036	0.04%	0.005%
59	10.786	3027	3031	3034	rVB5	1951	1447	0.06%	0.007%
60	10.831	3042	3045	3048	rBV5	1137	744	0.03%	0.004%
61	10.879	3057	3060	3062	rBV4	1417	733	0.03%	0.003%
62	10.898	3062	3066	3073	rBV10	1838	2642	0.10%	0.013%
63	10.972	3086	3089	3092	rBV4	1220	803	0.03%	0.004%
64	11.024	3103	3105	3109	rVB4	1699	1210	0.05%	0.006%
65	11.053	3109	3114	3119	rBV7	1392	1490	0.06%	0.007%
66	11.127	3133	3137	3138	rBV4	2260	1504	0.06%	0.007%
67	11.181	3143	3154	3180	rBV	1219865	1911556	72.70%	9.086%
68	11.423	3227	3229	3233	rBV5	1309	895	0.03%	0.004%
69	11.506	3248	3255	3257	rBV9	2633	2901	0.11%	0.014%
70	11.554	3259	3270	3300	rVV	1159885	1878071	71.43%	8.927%
71	11.953	3391	3394	3398	rBV5	1418	1257	0.05%	0.006%
72	12.191	3462	3468	3470	rBV4	4461	4473	0.17%	0.021%
73	12.265	3485	3491	3492	rBV6	1635	1221	0.05%	0.006%
74	12.320	3503	3508	3514	rBV8	1808	2683	0.10%	0.013%
75	12.368	3517	3523	3525	rBV7	1659	1580	0.06%	0.008%
76	12.406	3532	3535	3538	rVB5	1229	751	0.03%	0.004%

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 Title : VOC Analysis

77	12.423	3538	3540	3543	rBV2	1402	699	0.03%	0.003%
78	12.548	3576	3579	3580	rBV3	1250	757	0.03%	0.004%
79	12.590	3589	3592	3596	rVV6	1473	1330	0.05%	0.006%
80	12.670	3615	3617	3622	rBV5	921	828	0.03%	0.004%
81	12.792	3650	3655	3658	rBV5	1095	1015	0.04%	0.005%
82	12.866	3673	3678	3679	rBV4	1488	1163	0.04%	0.006%
83	12.947	3699	3703	3705	rBV5	1140	760	0.03%	0.004%
84	13.046	3729	3734	3735	rBV5	1537	1327	0.05%	0.006%
85	13.085	3740	3746	3747	rBV5	2488	1955	0.07%	0.009%
86	13.236	3790	3793	3798	rVB5	2307	1425	0.05%	0.007%
87	13.461	3859	3863	3866	rBV6	2440	2025	0.08%	0.010%
88	13.683	3929	3932	3936	rBV6	2283	1570	0.06%	0.007%
89	13.728	3942	3946	3949	rBV5	1331	969	0.04%	0.005%
90	13.840	3978	3981	3985	rVB5	2104	1235	0.05%	0.006%
91	13.860	3985	3987	3990	rBV4	1435	1164	0.04%	0.006%
92	13.988	4019	4027	4032	rVV5	3881	5220	0.20%	0.025%
93	14.107	4062	4064	4069	rBV6	1011	816	0.03%	0.004%
94	14.143	4071	4075	4077	rVV5	1768	1280	0.05%	0.006%
95	14.156	4077	4079	4083	rVB6	1583	1108	0.04%	0.005%
96	14.339	4132	4136	4146	rVB6	3980	5354	0.20%	0.025%
97	14.439	4162	4167	4169	rBV7	1685	1587	0.06%	0.008%
98	14.641	4228	4230	4232	rBV3	1395	708	0.03%	0.003%
99	14.718	4251	4254	4255	rBV3	1292	810	0.03%	0.004%
100	14.905	4311	4312	4320	rVB8	1306	1295	0.05%	0.006%

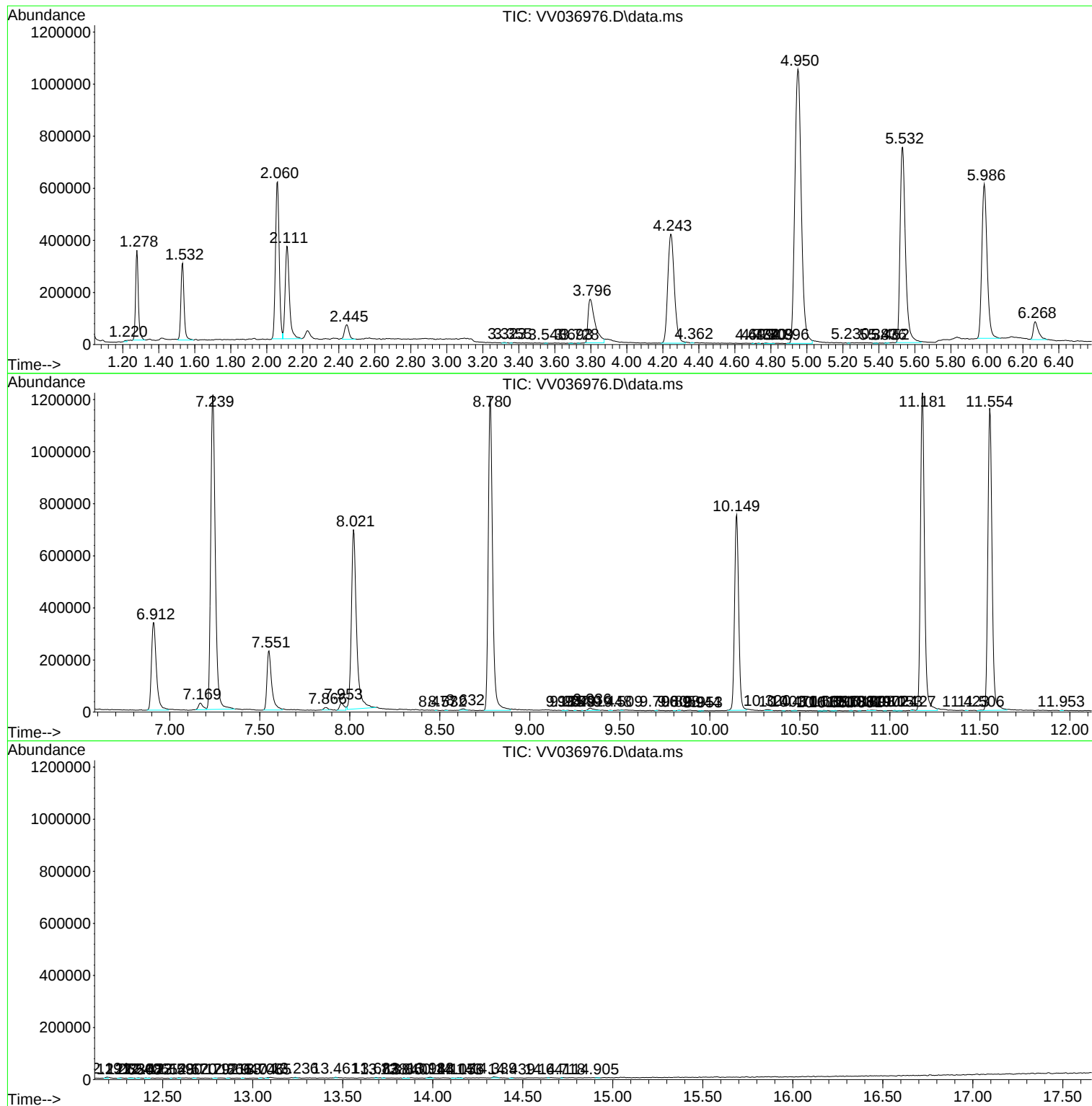
Sum of corrected areas: 21038593

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080224WMA.M
Quant Title : VOC Analysis

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



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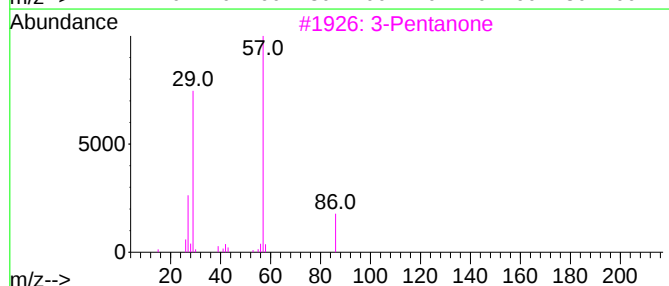
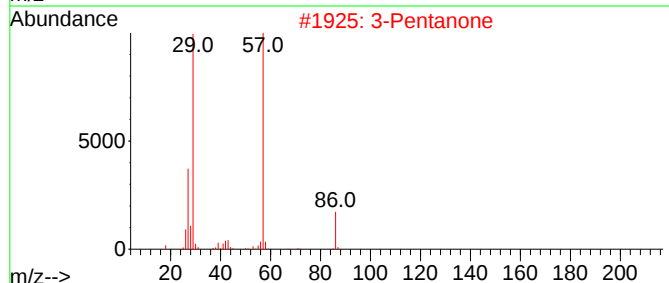
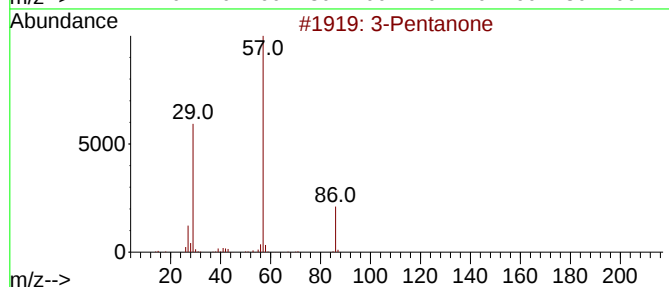
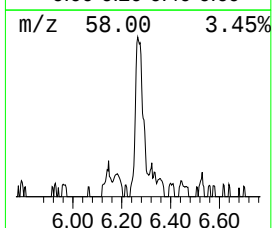
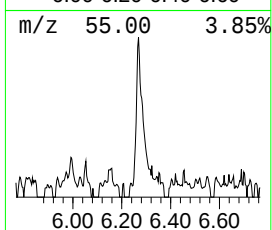
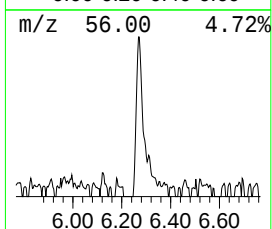
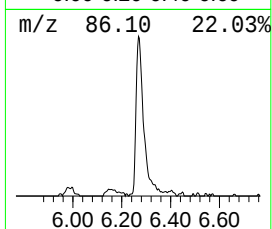
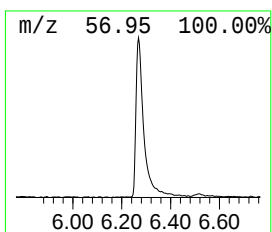
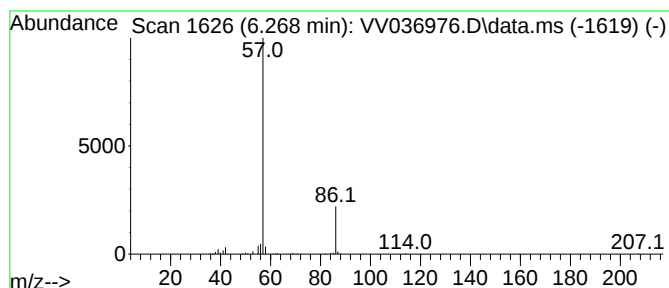
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM080224WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 3-Pentanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.268	4.35 ug/L	134835	1,4-Difluorobenzene	5.532

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Pentanone			86	C5H10O	000096-22-0	80
2	3-Pentanone			86	C5H10O	000096-22-0	72
3	3-Pentanone			86	C5H10O	000096-22-0	64
4	3-Pentanone			86	C5H10O	000096-22-0	59
5	Propanal, 2,2-dimethyl-			86	C5H10O	000630-19-3	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Pentanone	6.268	4.3	ug/L	134835	1	5.532	1551100	50.0