LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV101419\
Data File : VV013133.D
Acq On : 14 Oct 2019 11:27
Operator : SY/MD
Sample : VV1014MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : VBLK74

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\SOMVLM101119WMA.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	1.315	64	70	90	rVB	307906	328781	12.39%	1.666%
2	1.582	146	153	169	rVB	277123	320191	12.07%	1.622%
3	2.126	313	322	334	rBV	572736	796615	30.02%	4.036%
4	2.537	443	450	460	rVB4	4360	6675	0.25%	0.034%
5	2.794	520	530	536	rBV5	3106	5682	0.21%	0.029%
6	2.884	555	558	561	rVB3	896	564	0.02%	0.003%
7	2.910	561	566	569	rBV4	708	652	0.02%	0.003%
8	2.978	582	587	588	rBV3	516	470	0.02%	0.002%
9	3.026	595	602	604	rBV5	694	788	0.03%	0.004%
10	3.138	634	637	644	rVB3	587	480	0.02%	0.002%
11	3.183	649	651	654	rVB4	857	432	0.02%	0.002%
12	3.212	654	660	665	rBV4	705	902	0.03%	0.005%
13	3.261	672	675	681	rBV2	822	604	0.02%	0.003%
14	3.293	681	685	688	rBV	481	464	0.02%	0.002%
15	3.315	690	692	696	rVB2	715	440	0.02%	0.002%
16	3.370	705	709	712	rVV4	481	338	0.01%	0.002%
17	3.418	719	724	728	rVV4	975	808	0.03%	0.004%
18	3.605	775	782	786	rBV3	804	785	0.03%	0.004%
19	3.659	796	799	803	rVV3	517	368	0.01%	0.002%
20	3.746	821	826	829	rBV4	525	529	0.02%	0.003%
21	3.846	854	857	860	rVB2	616	389	0.01%	0.002%
22	3.868	860	864	867	rBV2	590	513	0.02%	0.003%
23	3.971	880	896	963	rBV	94316	608916	22.95%	3.085%
24	4.396	1012	1028	1058	rBV	415289	1015580	38.28%	5.145%
25	4.579	1081	1085	1090	rVB5	1075	1093	0.04%	0.006%
26	4.621	1095	1098	1101	rBV4	525	454	0.02%	0.002%
27	4.785	1146	1149	1152	rVB3	635	347	0.01%	0.002%
28	4.804	1152	1155	1157	rBV2	831	405	0.02%	0.002%
29	4.871	1170	1176	1178	rBV2	828	718	0.03%	0.004%
30	4.949	1196	1200	1201	rBV2	614	411	0.02%	0.002%
31	5.013	1217	1220	1225	rVB3	573	532	0.02%	0.003%
32	5.090	1225	1244	1289	rBV2	1066646	2653343	100.00%	13.443%
33	5.386	1334	1336	1339	rBV4	883	544	0.02%	0.003%
34	5.444	1351	1354	1356	rBV2	712	505	0.02%	0.003%

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ALS Vial : 3 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : VBLK74

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

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Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM101119WMA.M
Title : VOC Analysis

35	5.521	1373	1378	1379	rBV3	711	544	0.02%	0.003%
36	5.659	1406	1421	1452	rVV	894602	1773379	66.84%	8.985%
37	5.942	1496	1509	1530	rBV	60972	125941	4.75%	0.638%
38	6.113	1547	1562	1593	rBV	584663	1215175	45.80%	6.157%
39	6.325	1626	1628	1630	rVB3	853	356	0.01%	0.002%
40	6.341	1630	1633	1635	rBV2	981	645	0.02%	0.003%
41	6.408	1652	1654	1657	rBV3	955	507	0.02%	0.003%
42	6.463	1667	1671	1674	rBV2	633	578	0.02%	0.003%
43	6.547	1693	1697	1698	rBV2	518	330	0.01%	0.002%
44	6.637	1720	1725	1726	rBV4	760	548	0.02%	0.003%
45	6.862	1793	1795	1798	rBV2	457	347	0.01%	0.002%
46	6.932	1812	1817	1821	rBV3	530	557	0.02%	0.003%
47	6.958	1821	1825	1828	rBV	501	431	0.02%	0.002%
48	7.026	1832	1846	1872	rBV	298676	549240	20.70%	2.783%
49	7.267	1919	1921	1924	rVV3	799	567	0.02%	0.003%
50	7.283	1924	1926	1929	rVV4	1285	869	0.03%	0.004%
51	7.357	1936	1949	1968	rBV	1137875	1980480	74.64%	10.034%
52	7.662	2031	2044	2070	rBV	210773	370478	13.96%	1.877%
53	7.852	2100	2103	2106	rBV2	478	356	0.01%	0.002%
54	7.926	2123	2126	2129	rBV2	720	518	0.02%	0.003%
55	8.019	2145	2155	2163	rBV4	8020	14301	0.54%	0.072%
56	8.138	2179	2192	2226	rBV2	514168	1197936	45.15%	6.069%
57	8.495	2297	2303	2306	rBV5	676	712	0.03%	0.004%
58	8.672	2355	2358	2360	rBV2	622	448	0.02%	0.002%
59	8.698	2364	2366	2368	rBV3	600	327	0.01%	0.002%
60	8.891	2413	2426	2458	rBV	1311476	2155888	81.25%	10.923%
61	9.058	2471	2478	2485	rVB7	3051	4632	0.17%	0.023%
62	9.132	2496	2501	2502	rBV2	1392	964	0.04%	0.005%
63	9.183	2508	2517	2522	rBV7	2920	4490	0.17%	0.023%
64	9.264	2540	2542	2544	rBV	671	369	0.01%	0.002%
65	9.299	2548	2553	2557	rVB3	584	664	0.03%	0.003%
66	9.360	2568	2572	2576	rVV4	504	482	0.02%	0.002%
67	9.466	2602	2605	2608	rBV2	366	328	0.01%	0.002%
68	9.547	2627	2630	2633	rBV3	593	399	0.02%	0.002%
69	9.592	2633	2644	2648	rBV8	3190	5654	0.21%	0.029%
70	9.974	2755	2763	2769	rBV4	2829	4035	0.15%	0.020%
71	10.055	2785	2788	2793	rBV3	442	388	0.01%	0.002%

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ALS Vial : 3 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : VBLK74

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\SOMVLM101119WMA.M
Title : VOC Analysis

72	10.083	2793	2797	2801	rBV2	773	478	0.02%	0.002%
73	10.122	2805	2809	2811	rBV3	679	433	0.02%	0.002%
74	10.138	2811	2814	2819	rVB	431	436	0.02%	0.002%
75	10.257	2838	2851	2875	rBV	720304	1140786	42.99%	5.780%
76	10.411	2895	2899	2900	rBV	611	405	0.02%	0.002%
77	10.582	2946	2952	2962	rVB5	2620	3639	0.14%	0.018%
78	10.672	2977	2980	2982	rBV2	885	531	0.02%	0.003%
79	10.900	3045	3051	3055	rBV5	1059	1006	0.04%	0.005%
80	10.958	3061	3069	3076	rBV3	2527	3385	0.13%	0.017%
81	11.196	3139	3143	3145	rBV3	829	621	0.02%	0.003%
82	11.225	3145	3152	3160	rVV5	5298	7798	0.29%	0.040%
83	11.289	3160	3172	3196	rBV	1057359	1657705	62.48%	8.399%
84	11.582	3261	3263	3266	rBV2	550	398	0.01%	0.002%
85	11.669	3276	3290	3312	rBV	1055397	1683117	63.43%	8.527%
86	12.167	3439	3445	3446	rBV2	706	725	0.03%	0.004%
87	12.379	3507	3511	3513	rBV	502	432	0.02%	0.002%
88	12.466	3532	3538	3539	rBV4	910	857	0.03%	0.004%
89	12.624	3583	3587	3590	rBV3	827	725	0.03%	0.004%
90	12.694	3601	3609	3618	rVB6	6053	10254	0.39%	0.052%
91	12.733	3618	3621	3626	rBV	766	545	0.02%	0.003%
92	13.263	3783	3786	3788	rBV2	714	398	0.01%	0.002%
93	13.308	3792	3800	3811	rVB4	9648	14646	0.55%	0.074%
94	13.395	3823	3827	3830	rBV3	594	573	0.02%	0.003%
95	13.460	3845	3847	3849	rBV2	562	371	0.01%	0.002%
96	13.553	3867	3876	3887	rBV2	14635	25056	0.94%	0.127%
97	13.791	3943	3950	3960	rVB4	10885	16845	0.63%	0.085%
98	14.366	4127	4129	4133	rVB3	861	505	0.02%	0.003%
99	14.691	4228	4230	4236	rBV4	716	611	0.02%	0.003%
100	14.717	4236	4238	4241	rBV3	923	527	0.02%	0.003%

Sum of corrected areas: 19737989

LSC Report - Integrated Chromatogram

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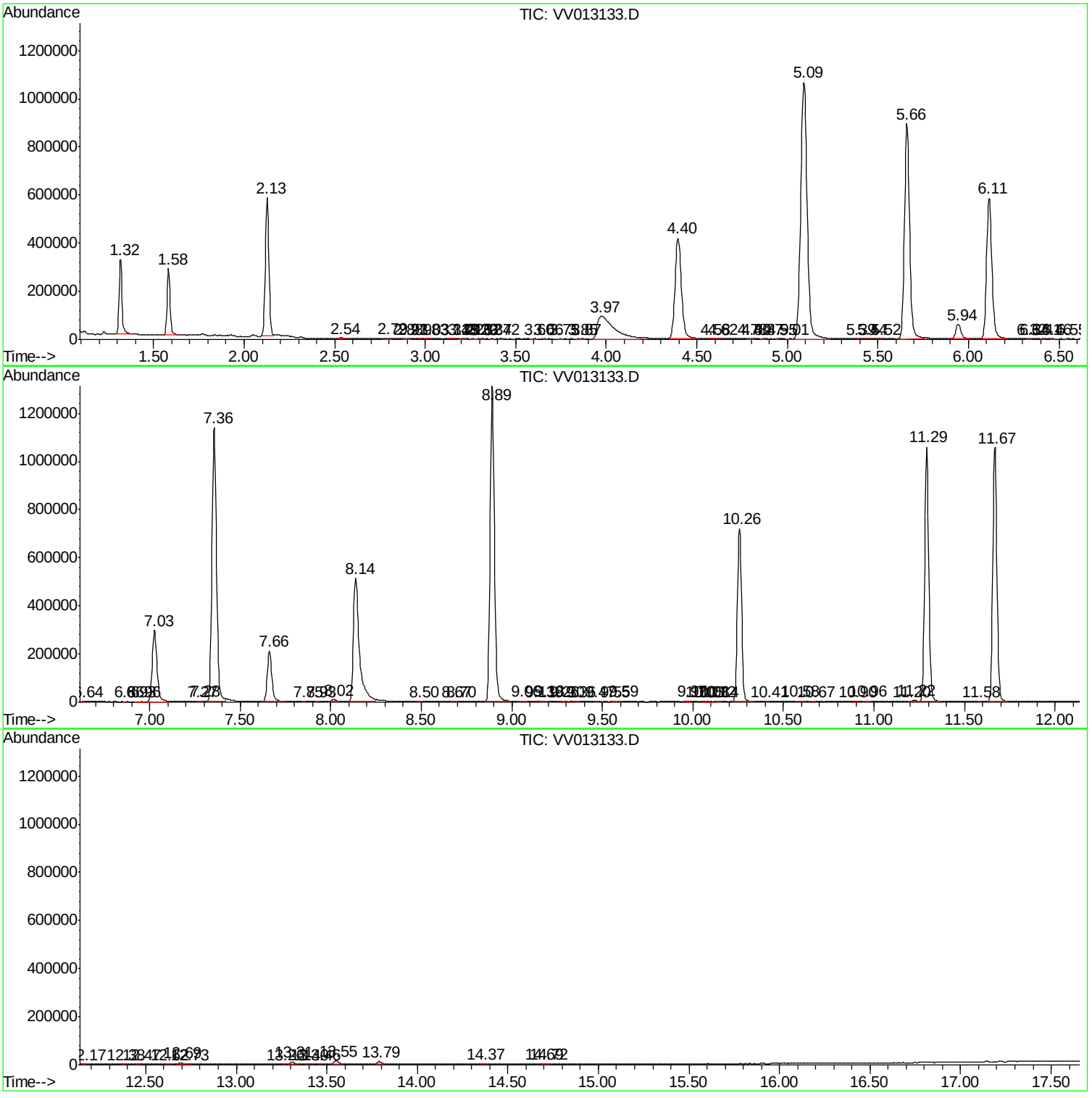
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : VBLK74

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM101119WMA.M
Quant Title : VOC Analysis

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV101419\
Data File : VV013133.D
Acq On : 14 Oct 2019 11:27
Operator : SY/MD
Sample : VV1014MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : VBLK74

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM101119WMA.M
Quant Title : VOC Analysis

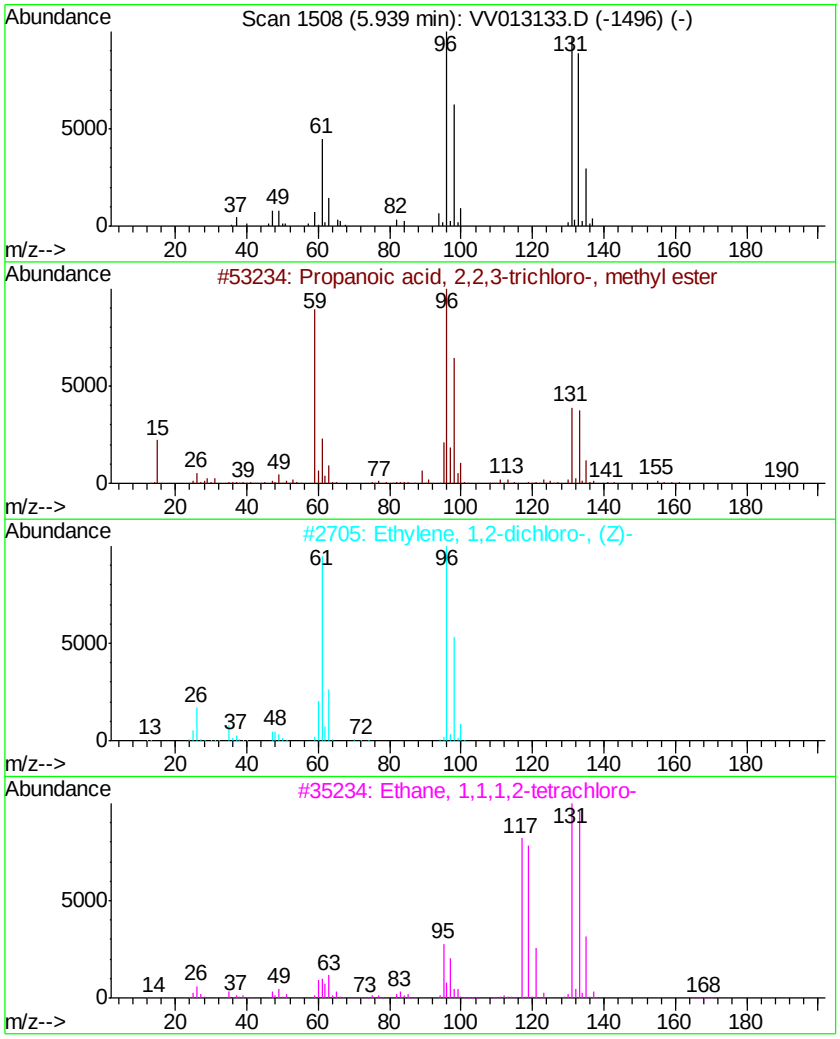
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

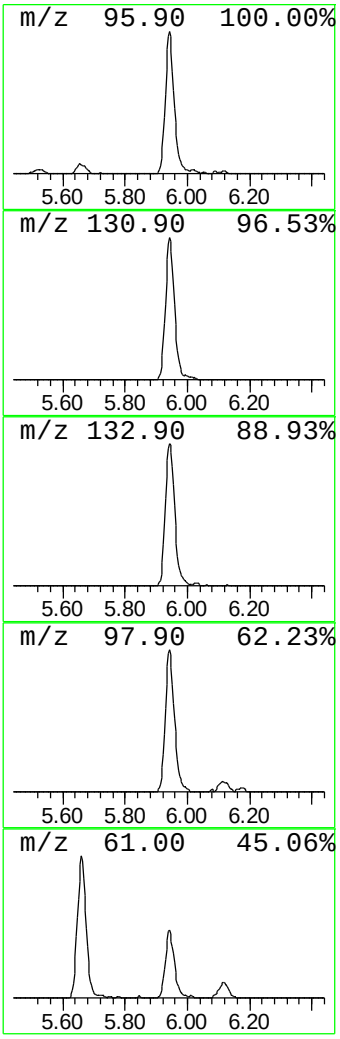
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.94	3.55 ug/L	125941	1,4-Difluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	56
2	Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
3	Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	23
4	m-Methoxybenzontrile	133	C8H7NO	001527-89-5	9
5	2-Cyano-3,5-dimethylpyrazine	133	C7H7N3	124629-52-3	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV101419\
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM101119WMA.M
Quant Title : VOC Analysis

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propanoic acid, 2...	5.94	3.5	ug/L	125941	1	5.66	1773380	50.0