LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV112919\
Data File : VV013844.D
Acq On : 29 Nov 2019 12:59
Operator : SY/MD
Sample : K6063-16ME
Misc : 6.04g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0BP3ME

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\SOMVLM110619WMA.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	1.200	29	34	46	rBV	120216	167237	6.98%	0.900%
2	1.315	64	70	89	rVB	256827	330842	13.81%	1.780%
3	2.103	306	315	325	rVB	539443	742468	30.99%	3.995%
4	2.904	561	564	565	rBV3	610	349	0.01%	0.002%
5	2.965	582	583	588	rVB5	1273	756	0.03%	0.004%
6	3.010	593	597	599	rBV4	1408	1100	0.05%	0.006%
7	3.103	624	626	630	rBV3	1051	606	0.03%	0.003%
8	3.193	652	654	657	rVB4	1283	602	0.03%	0.003%
9	3.248	667	671	673	rBV2	1267	1032	0.04%	0.006%
10	3.280	676	681	684	rVV8	1234	1198	0.05%	0.006%
11	3.296	684	686	691	rVV7	972	775	0.03%	0.004%
12	3.322	691	694	695	rVV2	1248	754	0.03%	0.004%
13	3.344	699	701	702	rBV2	992	379	0.02%	0.002%
14	3.354	702	704	706	rBV3	800	375	0.02%	0.002%
15	3.380	710	712	713	rBV2	952	383	0.02%	0.002%
16	3.441	729	731	735	rBV5	1857	1540	0.06%	0.008%
17	3.489	744	746	748	rVB3	1104	425	0.02%	0.002%
18	3.502	748	750	753	rBV2	1231	686	0.03%	0.004%
19	3.560	766	768	770	rBV2	905	548	0.02%	0.003%
20	3.592	777	778	780	rBV2	960	465	0.02%	0.003%
21	3.611	783	784	787	rBV3	661	338	0.01%	0.002%
22	3.637	787	792	794	rVB4	743	504	0.02%	0.003%
23	3.659	797	799	801	rVV3	936	444	0.02%	0.002%
24	3.743	823	825	828	rBV4	1005	660	0.03%	0.004%
25	3.782	835	837	841	rBV3	817	643	0.03%	0.003%
26	3.823	846	850	851	rVB4	1282	777	0.03%	0.004%
27	3.846	854	857	858	rBV3	1077	454	0.02%	0.002%
28	3.856	858	860	862	rBV2	892	400	0.02%	0.002%
29	3.872	862	865	866	rBV3	878	538	0.02%	0.003%
30	3.929	869	883	919	rBV	123562	442813	18.48%	2.383%
31	4.389	1007	1026	1049	rBV	390437	942747	39.35%	5.072%
32	4.675	1112	1115	1116	rBV3	1570	630	0.03%	0.003%
33	4.875	1172	1177	1182	rBV8	1414	1509	0.06%	0.008%
34	4.897	1182	1184	1188	rBV3	1346	852	0.04%	0.005%

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Misc : 6.04g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0BP3ME

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\SOMVLM110619WMA.M
Title : VOC Analysis

35	4.952	1199	1201	1204	rBV3	1199	752	0.03%	0.004%
36	5.010	1215	1219	1221	rVB5	1527	1031	0.04%	0.006%
37	5.084	1221	1242	1273	rBV2	965892	2395833	100.00%	12.891%
38	5.598	1396	1402	1403	rBV2	18618	15447	0.64%	0.083%
39	5.653	1409	1419	1447	rVB	735159	1466040	61.19%	7.888%
40	6.109	1549	1561	1591	rVB	521722	1069236	44.63%	5.753%
41	6.515	1683	1687	1688	rBV4	2002	1373	0.06%	0.007%
42	7.023	1834	1845	1865	rBV	274947	508050	21.21%	2.734%
43	7.354	1936	1948	1966	rBV	1114030	1943496	81.12%	10.457%
44	7.659	2032	2043	2062	rBV	184909	351431	14.67%	1.891%
45	8.068	2167	2170	2174	rBV5	2351	2117	0.09%	0.011%
46	8.138	2179	2192	2226	rBV	521193	1153359	48.14%	6.206%
47	8.498	2302	2304	2306	rBV2	1404	663	0.03%	0.004%
48	8.553	2319	2321	2323	rBV2	1236	617	0.03%	0.003%
49	8.695	2359	2365	2370	rBV9	4179	6145	0.26%	0.033%
50	8.785	2391	2393	2396	rBV4	1025	672	0.03%	0.004%
51	8.891	2414	2426	2449	rBV	1048703	1814512	75.74%	9.763%
52	9.138	2500	2503	2507	rBV4	2438	2099	0.09%	0.011%
53	9.350	2566	2569	2570	rBV3	1664	610	0.03%	0.003%
54	9.360	2570	2572	2574	rVV3	1448	561	0.02%	0.003%
55	9.486	2608	2611	2612	rBV4	1385	630	0.03%	0.003%
56	9.534	2625	2626	2627	rBV	952	358	0.01%	0.002%
57	9.576	2636	2639	2640	rBV3	2450	1462	0.06%	0.008%
58	9.772	2698	2700	2702	rBV3	1189	512	0.02%	0.003%
59	9.813	2710	2713	2716	rBV4	1890	1520	0.06%	0.008%
60	9.891	2730	2737	2744	rBV10	2900	3509	0.15%	0.019%
61	9.952	2753	2756	2763	rBV7	3014	3403	0.14%	0.018%
62	9.997	2768	2770	2771	rBV2	1129	417	0.02%	0.002%
63	10.019	2776	2777	2779	rBV2	920	423	0.02%	0.002%
64	10.109	2801	2805	2808	rBV3	1437	1371	0.06%	0.007%
65	10.260	2839	2852	2870	rBV	789126	1284307	53.61%	6.910%
66	10.463	2913	2915	2917	rBV3	1330	633	0.03%	0.003%
67	10.476	2917	2919	2920	rBV2	1102	443	0.02%	0.002%
68	10.527	2933	2935	2939	rBV4	1024	597	0.02%	0.003%
69	10.547	2939	2941	2944	rBV4	1226	794	0.03%	0.004%
70	10.572	2947	2949	2953	rVB5	1378	740	0.03%	0.004%
71	10.588	2953	2954	2956	rBV3	930	406	0.02%	0.002%

LSC Area Percent Report

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Misc : 6.04g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0BP3ME

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\SOMVLM110619WMA.M
Title : VOC Analysis

72	10.659	2974	2976	2978	rBV3	1020	483	0.02%	0.003%
73	10.794	3015	3018	3021	rBV4	1173	790	0.03%	0.004%
74	10.810	3021	3023	3028	rVB4	1680	1065	0.04%	0.006%
75	10.833	3028	3030	3031	rBV2	900	428	0.02%	0.002%
76	10.887	3045	3047	3048	rBV2	1620	546	0.02%	0.003%
77	10.897	3048	3050	3051	rBV2	1349	511	0.02%	0.003%
78	10.961	3064	3070	3072	rBV6	2230	2078	0.09%	0.011%
79	11.000	3080	3082	3084	rBV3	1141	612	0.03%	0.003%
80	11.084	3106	3108	3109	rBV2	1120	482	0.02%	0.003%
81	11.135	3123	3124	3126	rBV2	1158	385	0.02%	0.002%
82	11.196	3140	3143	3145	rBV3	1720	1119	0.05%	0.006%
83	11.293	3160	3173	3191	rBV	1198808	1865425	77.86%	10.037%
84	11.669	3277	3290	3310	rBV	1279698	2014807	84.10%	10.841%
85	12.051	3408	3409	3413	rBV3	1561	803	0.03%	0.004%
86	12.119	3428	3430	3432	rBV3	1106	527	0.02%	0.003%
87	12.402	3514	3518	3520	rBV5	2215	1721	0.07%	0.009%
88	12.521	3554	3555	3558	rBV3	972	465	0.02%	0.003%
89	12.656	3594	3597	3601	rBV4	2111	1920	0.08%	0.010%
90	12.691	3606	3608	3611	rBV3	2264	1375	0.06%	0.007%
91	12.823	3646	3649	3651	rBV3	2181	1157	0.05%	0.006%
92	12.910	3672	3676	3677	rBV2	1802	1246	0.05%	0.007%
93	12.958	3689	3691	3694	rBV4	1927	1184	0.05%	0.006%
94	13.029	3712	3713	3714	rBV	1663	567	0.02%	0.003%
95	13.196	3763	3765	3768	rBV3	919	674	0.03%	0.004%
96	13.247	3777	3781	3783	rBV4	1914	1655	0.07%	0.009%
97	13.733	3930	3932	3933	rBV2	1081	406	0.02%	0.002%
98	13.765	3940	3942	3943	rBV	1196	400	0.02%	0.002%
99	14.080	4038	4040	4043	rBV4	944	561	0.02%	0.003%
100	14.540	4181	4183	4185	rBV3	2110	833	0.03%	0.004%

Sum of corrected areas: 18585623

LSC Report - Integrated Chromatogram

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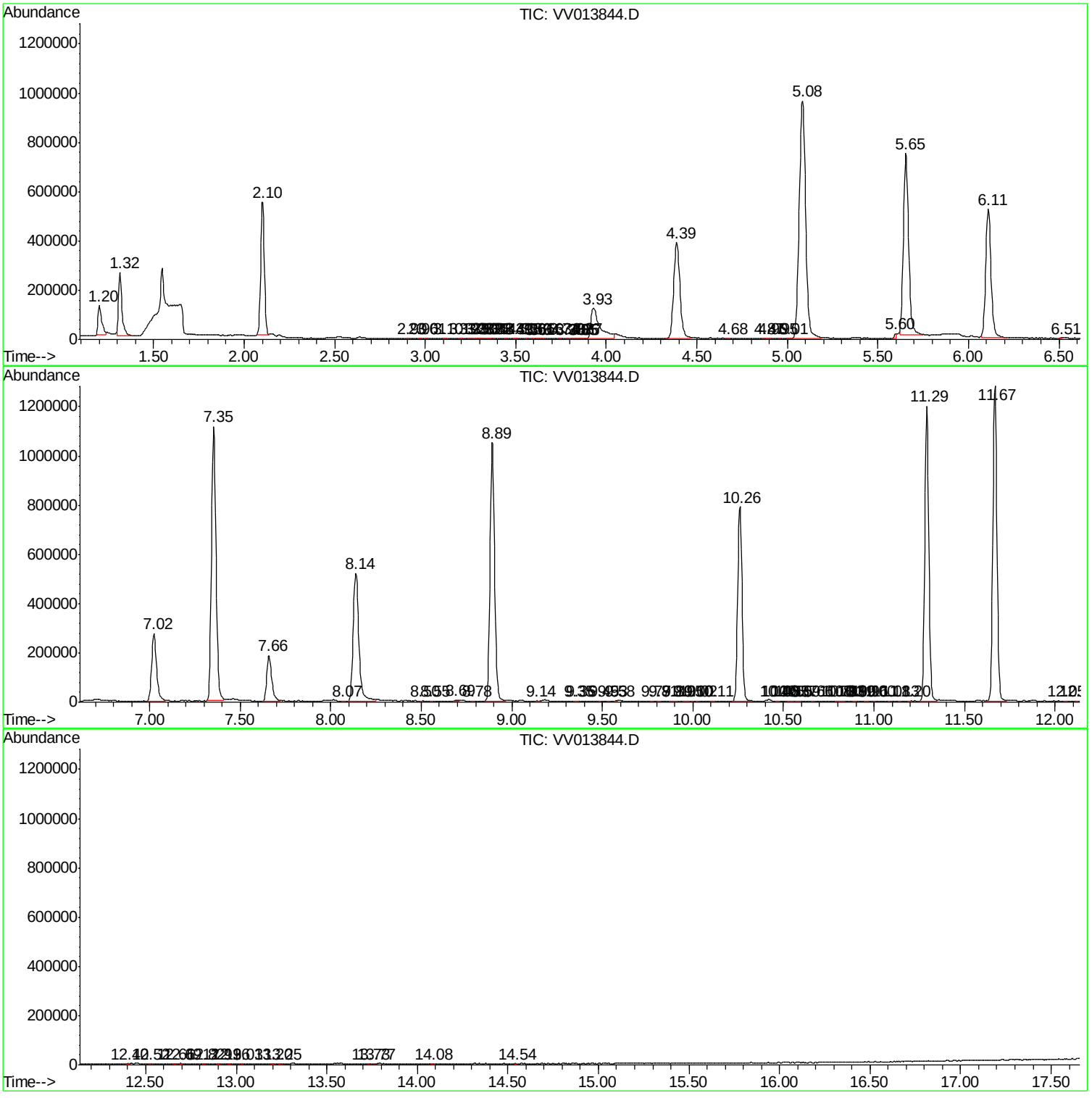
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0BP3ME

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM110619WMA.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\VV112919\
Data File : VV013844.D
Acq On : 29 Nov 2019 12:59
Operator : SY/MD
Sample : K6063-16ME
Misc : 6.04g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 9 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0BP3ME

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM110619WMA.M
Quant Title : VOC Analysis

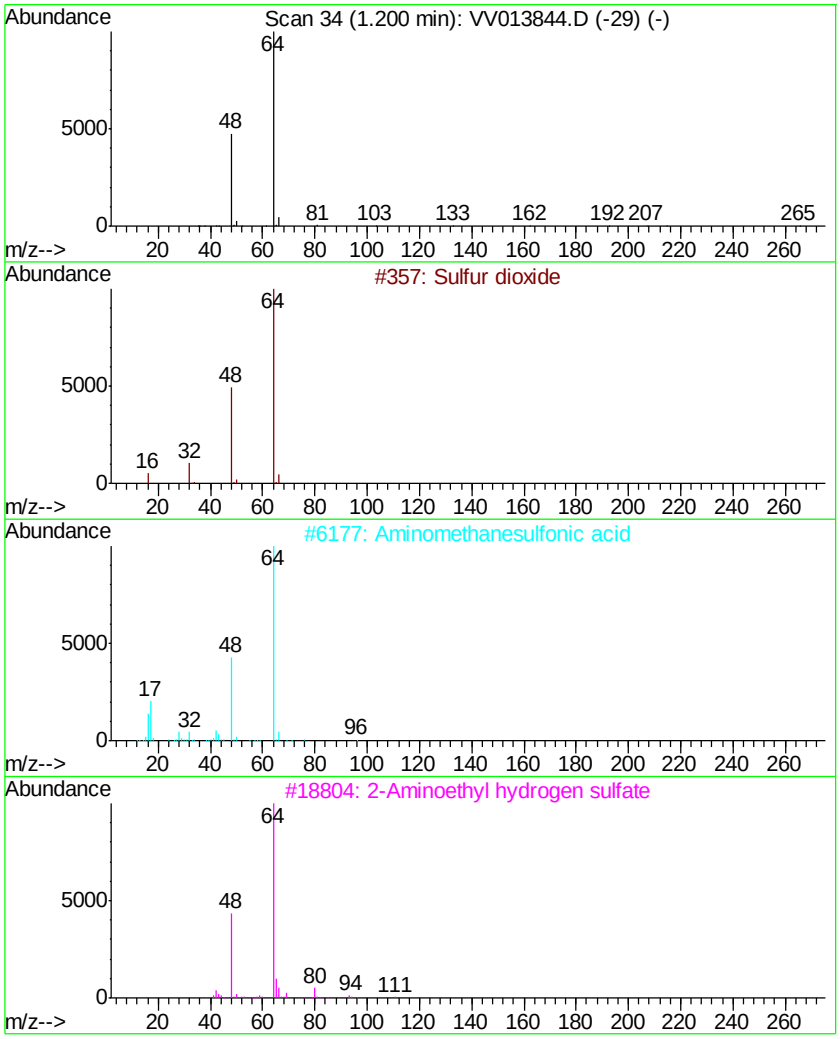
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

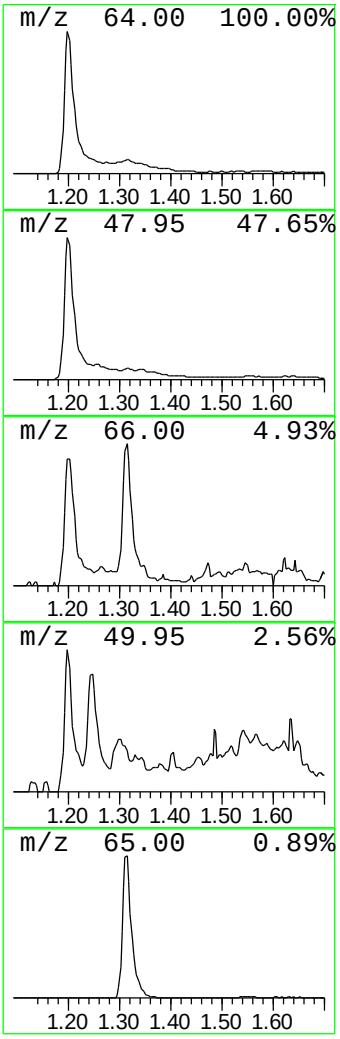
****

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.20	5.70 ug/L	167237	1,4-Difluorobenzene	5.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3	2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	4,6-Diamino-5-pyrimidinyl hydrog...	206	C4H6N4O4S	071525-41-2	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV112919\
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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
Sulfur dioxide	1.20	5.7	ug/L	167237	1	5.65	1466040	50.0