

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU100421\
 Data File : VU045097.D
 Acq On : 04 Oct 2021 15:35
 Operator : SY/MD
 Sample : M3996-05
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F4A17

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_U\Method\SFAMULM092321WMA.M
 Title : VOC Analysis

Signal : TIC: VU045097.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.476	34	42	60	rBV	30603	82412	6.31%	0.724%
2	1.601	75	81	95	rBV	152112	175752	13.45%	1.543%
3	1.906	168	176	192	rVB	121360	166861	12.77%	1.465%
4	2.469	343	351	362	rVB2	10055	15725	1.20%	0.138%
5	2.569	369	382	397	rBV	240956	398547	30.49%	3.499%
6	2.797	446	453	464	rBV3	1236	2505	0.19%	0.022%
7	2.958	496	503	505	rBV2	716	876	0.07%	0.008%
8	3.025	516	524	527	rBV4	1146	1640	0.13%	0.014%
9	3.083	539	542	546	rVB4	704	581	0.04%	0.005%
10	3.141	549	560	565	rBV5	1169	1775	0.14%	0.016%
11	3.193	568	576	591	rVV2	3968	8685	0.66%	0.076%
12	3.363	620	629	642	rBV5	2658	4777	0.37%	0.042%
13	3.575	693	695	698	rVB2	344	208	0.02%	0.002%
14	3.701	731	734	741	rVB2	340	363	0.03%	0.003%
15	3.984	815	822	827	rBV4	762	1014	0.08%	0.009%
16	4.160	871	877	880	rBV2	190	237	0.02%	0.002%
17	4.328	925	929	930	rBV2	356	218	0.02%	0.002%
18	4.527	984	991	992	rBV3	1208	993	0.08%	0.009%
19	4.627	1007	1022	1060	rBV	164868	393534	30.11%	3.455%
20	4.823	1079	1083	1086	rBV3	263	280	0.02%	0.002%
21	4.948	1118	1122	1126	rBV2	229	273	0.02%	0.002%
22	5.067	1142	1159	1185	rBV	227611	502924	38.48%	4.416%
23	5.186	1192	1196	1202	rVB3	558	624	0.05%	0.005%
24	5.289	1221	1228	1236	rBV4	655	1141	0.09%	0.010%
25	5.382	1252	1257	1259	rBV	612	515	0.04%	0.005%
26	5.398	1259	1262	1266	rVB	403	306	0.02%	0.003%
27	5.469	1282	1284	1289	rVB3	340	253	0.02%	0.002%
28	5.508	1289	1296	1297	rBV	208	263	0.02%	0.002%
29	5.627	1329	1333	1339	rVB	157	214	0.02%	0.002%
30	5.729	1343	1365	1394	rBV2	457772	1306998	100.00%	11.475%
31	5.890	1411	1415	1417	rBV3	369	258	0.02%	0.002%
32	6.032	1452	1459	1462	rVB3	256	299	0.02%	0.003%
33	6.115	1480	1485	1486	rBV3	353	250	0.02%	0.002%
34	6.160	1495	1499	1501	rBV2	349	244	0.02%	0.002%
35	6.254	1512	1528	1547	rVV	384068	712512	54.52%	6.256%
36	6.376	1563	1566	1571	rVB4	571	472	0.04%	0.004%

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 Title : VOC Analysis

37	6.411	1571	1577	1578	rBV2	322	293	0.02%	0.003%
38	6.479	1593	1598	1603	rBV2	217	320	0.02%	0.003%
39	6.543	1606	1618	1633	rVB8	4984	9629	0.74%	0.085%
40	6.601	1633	1636	1639	rBV2	297	269	0.02%	0.002%
41	6.694	1651	1665	1691	rBV	299249	582802	44.59%	5.117%
42	6.797	1695	1697	1698	rVV	466	249	0.02%	0.002%
43	6.807	1698	1700	1706	rVV3	785	683	0.05%	0.006%
44	6.884	1720	1724	1726	rBV	263	186	0.01%	0.002%
45	6.945	1741	1743	1747	rVB2	241	188	0.01%	0.002%
46	6.971	1747	1751	1754	rBV2	218	184	0.01%	0.002%
47	7.048	1768	1775	1779	rBV2	558	683	0.05%	0.006%
48	7.067	1779	1781	1784	rVB	285	202	0.02%	0.002%
49	7.112	1784	1795	1805	rBV2	5292	8982	0.69%	0.079%
50	7.186	1805	1818	1827	rBV8	2515	4731	0.36%	0.042%
51	7.569	1924	1937	1953	rBV	166609	286733	21.94%	2.518%
52	7.688	1967	1974	1984	rVB3	1977	2994	0.23%	0.026%
53	7.742	1987	1991	1994	rVB3	244	213	0.02%	0.002%
54	7.797	2003	2008	2010	rBV2	210	210	0.02%	0.002%
55	7.900	2026	2040	2054	rBV	539845	926849	70.91%	8.138%
56	7.974	2054	2063	2082	rVB	45910	78836	6.03%	0.692%
57	8.183	2116	2128	2152	rBV	114670	191238	14.63%	1.679%
58	8.360	2179	2183	2188	rBV2	212	184	0.01%	0.002%
59	8.479	2210	2220	2229	rVB4	1009	1948	0.15%	0.017%
60	8.556	2230	2244	2258	rBV	666022	1130840	86.52%	9.929%
61	8.636	2258	2269	2302	rVB	516488	876338	67.05%	7.694%
62	8.906	2350	2353	2360	rVV2	210	223	0.02%	0.002%
63	8.990	2376	2379	2386	rVV2	245	370	0.03%	0.003%
64	9.138	2420	2425	2428	rBV	159	185	0.01%	0.002%
65	9.279	2465	2469	2472	rBV	186	201	0.02%	0.002%
66	9.421	2499	2513	2550	rBV	524731	865268	66.20%	7.597%
67	9.572	2550	2560	2571	rBV	18222	28053	2.15%	0.246%
68	9.700	2588	2600	2613	rVB2	17938	29306	2.24%	0.257%
69	9.970	2679	2684	2687	rBV2	250	290	0.02%	0.003%
70	10.106	2715	2726	2737	rBV2	11076	17207	1.32%	0.151%
71	10.244	2762	2769	2775	rBV2	279	493	0.04%	0.004%
72	10.488	2838	2845	2849	rBV	395	487	0.04%	0.004%
73	10.671	2896	2902	2914	rVB3	1440	2116	0.16%	0.019%
74	10.761	2917	2930	2948	rVV	433584	697170	53.34%	6.121%
75	10.848	2953	2957	2960	rBV2	275	299	0.02%	0.003%
76	10.871	2962	2964	2968	rVV2	333	315	0.02%	0.003%

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 Title : VOC Analysis

77	10.906	2968	2975	2985	rVB2	2447	3798	0.29%	0.033%
78	11.003	2996	3005	3009	rBV2	3150	4408	0.34%	0.039%
79	11.093	3027	3033	3038	rVB2	1213	1304	0.10%	0.011%
80	11.295	3089	3096	3104	rBV2	1864	2606	0.20%	0.023%
81	11.469	3140	3150	3167	rBV	12573	19312	1.48%	0.170%
82	11.697	3217	3221	3227	rVB3	964	1007	0.08%	0.009%
83	11.813	3245	3257	3276	rBV	517569	817350	62.54%	7.176%
84	11.896	3280	3283	3292	rVB3	1901	2210	0.17%	0.019%
85	11.974	3303	3307	3316	rVB3	1456	1664	0.13%	0.015%
86	12.044	3324	3329	3334	rBV	330	416	0.03%	0.004%
87	12.096	3338	3345	3354	rVV3	4324	6380	0.49%	0.056%
88	12.195	3361	3376	3392	rBV	540253	868633	66.46%	7.627%
89	12.575	3488	3494	3502	rBV4	981	1452	0.11%	0.013%
90	12.687	3524	3529	3536	rVB3	424	577	0.04%	0.005%
91	13.031	3628	3636	3647	rBV3	847	1332	0.10%	0.012%
92	13.189	3682	3685	3690	rBV	303	340	0.03%	0.003%
93	13.263	3705	3708	3714	rBV2	282	286	0.02%	0.003%
94	13.298	3714	3719	3723	rBV2	872	907	0.07%	0.008%
95	13.459	3763	3769	3776	rVB4	1454	2089	0.16%	0.018%
96	14.089	3955	3965	3979	rBV	30911	50911	3.90%	0.447%
97	14.211	3995	4003	4015	rVB2	3827	5553	0.42%	0.049%
98	15.176	4295	4303	4308	rBV3	1210	1683	0.13%	0.015%
99	15.227	4309	4319	4339	rVB	19621	34446	2.64%	0.302%
100	15.414	4367	4377	4392	rVB3	16590	28520	2.18%	0.250%

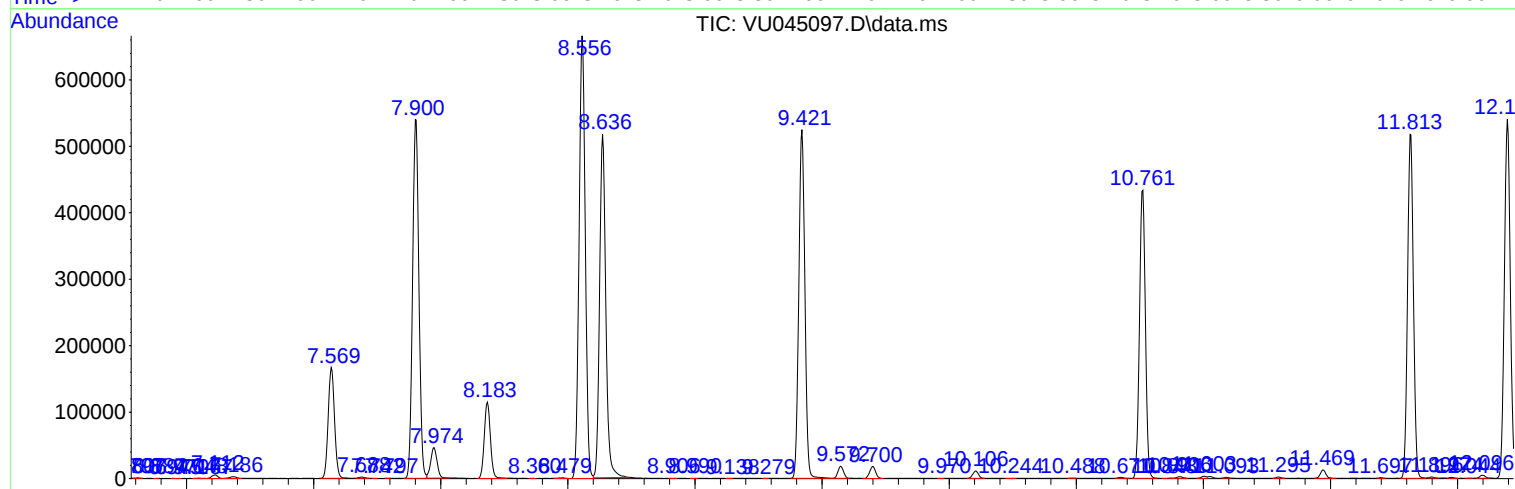
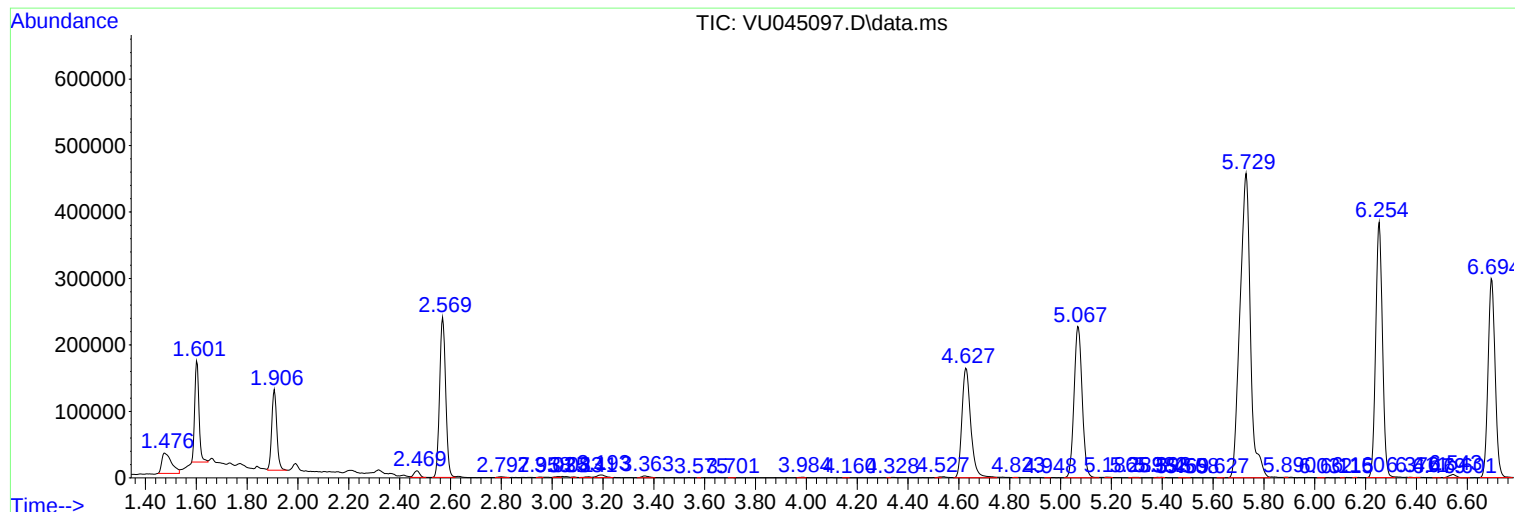
Sum of corrected areas: 11389480

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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



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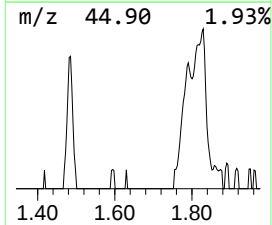
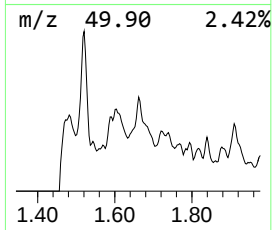
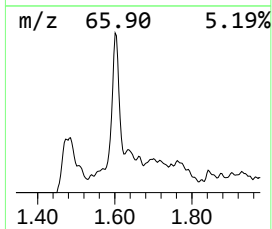
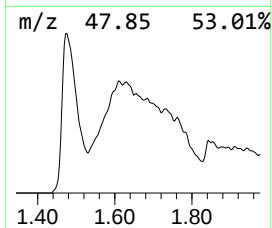
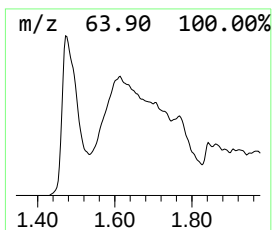
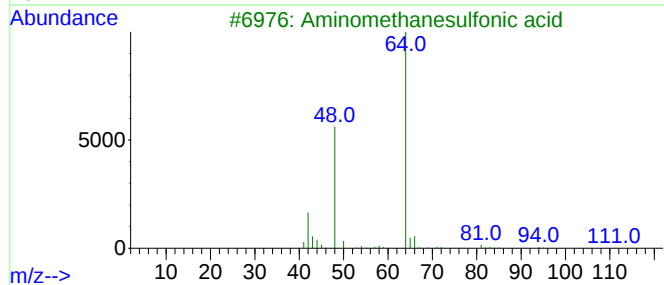
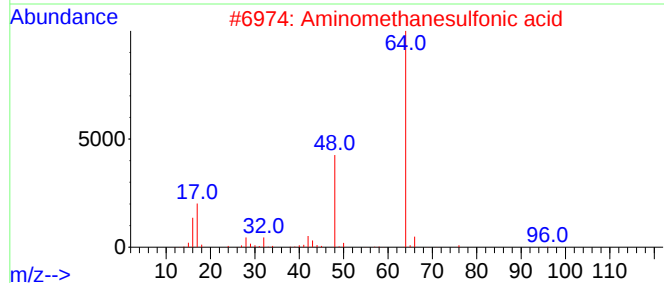
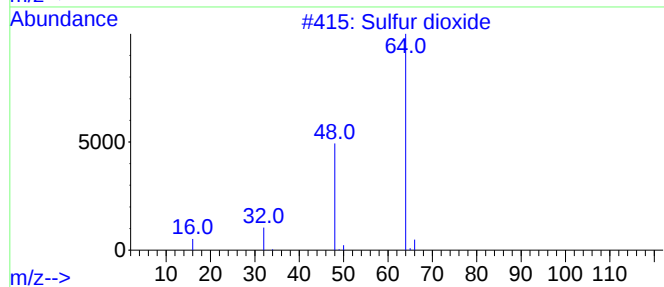
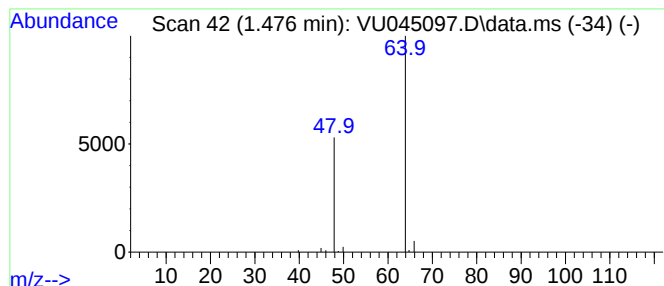
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.476	5.78 ug/L	82412	1,4-Difluorobenzene	6.254

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			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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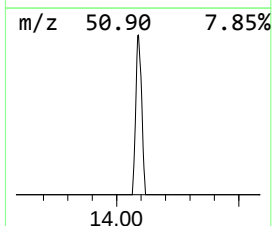
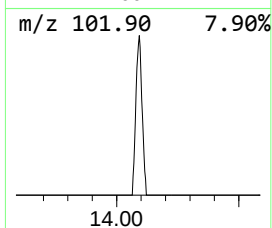
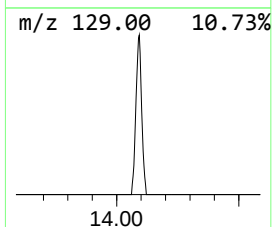
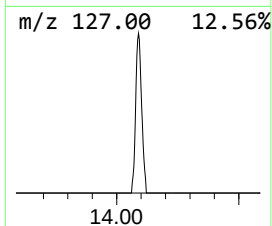
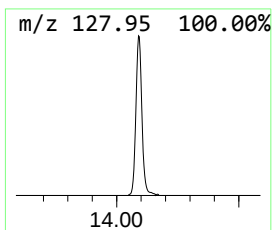
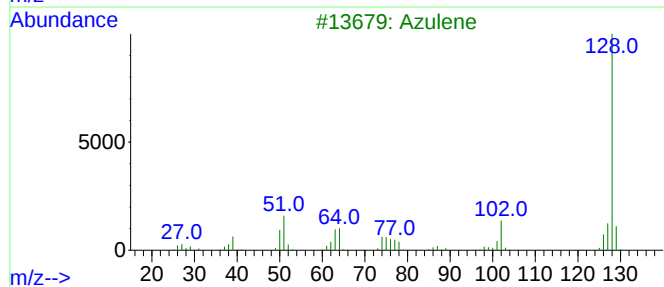
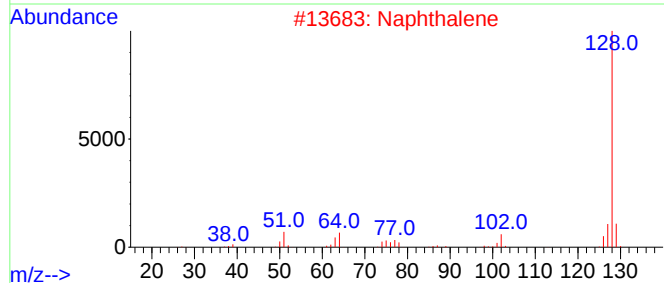
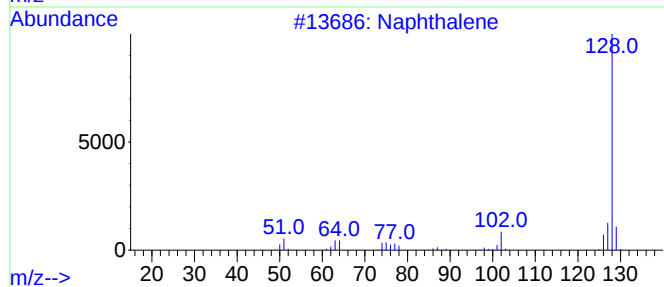
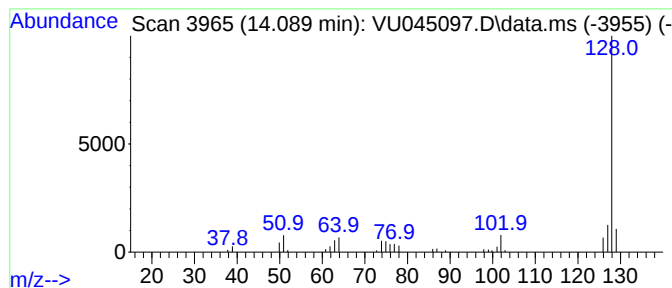
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092321WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.089	3.11 ug/L	50911	1,4-Dichlorobenzene-d4	11.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Naphthalene	128	C10H8	000091-20-3	94
3			Azulene	128	C10H8	000275-51-4	91
4			Azulene	128	C10H8	000275-51-4	91
5			Naphthalene	128	C10H8	000091-20-3	91



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Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.476	5.8	ug/L	82412	1	6.254	712512	50.0
Azulene	14.089	3.1	ug/L	50911	3	11.816	817350	50.0