

Average, standard deviation, and standard error values for each timepoint in measured metabolites from the 2010 green berry incorporation trial

Supplementary Table 1

Mean values of								
Sampling dates	Phenylalanine [M+6]	Phenylalanine	caftaric acid	c-coutaric acid	c-coutaric acid [M+6]	t-coutaric acid [M+6]	t-coutaric acid	
7/27/2010	0.000	40.579	283.966	81.894	0.000	0.000	24.339	
7/29/2010	12.118	36.244	265.134	77.934	0.000	0.000	24.275	
7/30/2010	4.577	36.022	333.219	114.144	0.000	0.000	30.008	
8/1/2010	1.853	17.725	236.181	77.512	0.000	0.000	21.146	
8/5/2010	0.807	17.030	218.795	77.040	0.000	0.000	25.786	
8/13/2010	0.300	7.296	81.003	25.425	0.009	0.004	20.063	
8/17/2010	0.355	11.812	65.096	12.725	0.001	0.007	17.334	
8/26/2010	0.735	27.837	33.657	2.931	0.000	0.007	10.764	
9/9/2010	0.614	21.223	14.660	0.119	0.000	0.007	8.432	
Stdev	Phenylalanine [M+6]	Phenylalanine	caftaric acid	c-coutaric acid	c-coutaric acid [M+6]	t-coutaric acid [M+6]	t-coutaric acid	
7/27/2010	0.000	12.853	111.983	33.974	0.000	0.000	7.691	
7/29/2010	5.612	16.089	98.247	31.136	0.000	0.000	9.037	
7/30/2010	3.268	12.824	66.179	26.479	0.000	0.000	5.879	
8/1/2010	1.482	8.839	60.034	23.503	0.000	0.000	5.220	
8/5/2010	0.442	10.510	48.220	17.242	0.000	0.000	4.184	
8/13/2010	0.128	2.950	45.240	13.519	0.012	0.006	4.104	
8/17/2010	0.171	4.521	26.126	5.572	0.004	0.006	2.787	
8/26/2010	0.274	6.671	8.545	1.474	0.000	0.006	2.318	
9/9/2010	0.419	8.466	5.615	0.192	0.000	0.007	2.609	
StErr	Phenylalanine [M+6]	Phenylalanine	caftaric acid	c-coutaric acid	c-coutaric acid [M+6]	t-coutaric acid [M+6]	t-coutaric acid	
7/27/2010	0.000	3.710	32.327	9.808	0.000	0.000	2.220	
7/29/2010	1.620	4.644	28.361	8.988	0.000	0.000	2.609	
7/30/2010	0.943	3.702	19.104	7.644	0.000	0.000	1.697	
8/1/2010	0.428	2.552	17.330	6.785	0.000	0.000	1.507	
8/5/2010	0.127	3.034	13.920	4.977	0.000	0.000	1.208	
8/13/2010	0.037	0.851	13.060	3.903	0.003	0.002	1.185	
8/17/2010	0.049	1.305	7.542	1.608	0.001	0.002	0.805	
8/26/2010	0.079	1.926	2.467	0.425	0.000	0.002	0.669	
9/9/2010	0.121	2.444	1.621	0.055	0.000	0.002	0.753	

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Mean values of								
Sampling dates		Myr-3-Glucuronide [M+6]	Myr-3-Glucuronide	Myr-3-Glucoside [M+6]	Myr-3-Glucoside	Q-3-Glucuronide	Q-3-Glucoside [M+6]	
7/27/2010		0.000	1.107	0.000	0.141	96.995	0.000	
7/29/2010		0.000	0.948	0.000	0.042	83.880	0.090	
7/30/2010		0.000	0.906	0.000	0.124	60.385	0.060	
8/1/2010		0.000	0.545	0.000	0.018	51.957	0.118	
8/5/2010		0.000	2.645	0.000	3.391	78.235	0.391	
8/13/2010		0.008	4.852	0.011	29.740	96.665	0.242	
8/17/2010		0.005	5.410	0.031	46.084	108.729	0.212	
8/26/2010		0.011	10.988	0.113	81.730	171.526	0.454	
9/9/2010		0.008	7.915	0.065	82.378	114.205	0.194	
Stdev		Myr-3-Glucuronide [M+6]	Myr-3-Glucuronide	Myr-3-Glucoside [M+6]	Myr-3-Glucoside	Q-3-Glucuronide	Q-3-Glucoside [M+6]	
7/27/2010		0.000	0.747	0.000	0.210	52.249	0.000	
7/29/2010		0.000	0.744	0.000	0.079	44.805	0.097	
7/30/2010		0.000	0.600	0.000	0.163	36.459	0.074	
8/1/2010		0.000	0.359	0.000	0.043	25.447	0.113	
8/5/2010		0.000	1.466	0.000	2.383	40.610	0.328	
8/13/2010		0.009	3.592	0.024	21.918	58.862	0.193	
8/17/2010		0.004	3.379	0.031	24.658	65.376	0.168	
8/26/2010		0.007	3.813	0.090	24.469	30.521	0.278	
9/9/2010		0.005	2.809	0.041	44.186	75.041	0.127	
StErr		Myr-3-Glucuronide [M+6]	Myr-3-Glucuronide	Myr-3-Glucoside [M+6]	Myr-3-Glucoside	Q-3-Glucuronide	Q-3-Glucoside [M+6]	
7/27/2010		0.000	0.216	0.000	0.060	15.083	0.000	
7/29/2010		0.000	0.215	0.000	0.023	12.934	0.028	
7/30/2010		0.000	0.173	0.000	0.047	10.525	0.021	
8/1/2010		0.000	0.104	0.000	0.013	7.346	0.033	
8/5/2010		0.000	0.423	0.000	0.688	11.723	0.095	
8/13/2010		0.003	1.037	0.007	6.327	16.992	0.056	
8/17/2010		0.001	0.975	0.009	7.118	18.872	0.049	
8/26/2010		0.002	1.101	0.026	7.064	8.811	0.080	
9/9/2010		0.001	0.811	0.012	12.755	21.662	0.037	

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Supplementary Table 1

Mean values of									
Sampling dates	Q-3-Glucoside	L-3-Glucoside	K-3-Galactoside	K-3-Glucoside [M+6]	K-3-Glucoside	I-3-Glucoside	Dp-3-Glucoside [M+6]		
7/27/2010	15.774	0.009	0.001	0.000	0.000	0.405	0.000	0.000	0.000
7/29/2010	13.505	0.000	0.000	0.000	0.000	0.237	0.000	0.000	0.000
7/30/2010	8.869	0.000	0.000	0.000	0.000	0.103	0.000	0.000	0.000
8/1/2010	8.397	0.000	0.000	0.000	0.000	0.105	0.000	0.000	0.000
8/5/2010	22.339	0.040	0.097	0.000	0.000	0.997	0.310	0.207	0.207
8/13/2010	63.174	1.831	1.920	0.016	0.016	7.190	7.322	0.305	0.305
8/17/2010	89.012	3.626	2.996	0.020	0.020	11.021	13.301	0.357	0.357
8/26/2010	153.267	10.376	4.396	0.031	0.031	26.813	27.883	0.392	0.392
9/9/2010	135.870	14.606	5.101	0.012	0.012	24.287	29.754	0.300	0.300
Stdev	Q-3-Glucoside	L-3-Glucoside	K-3-Galactoside	K-3-Glucoside [M+6]	K-3-Glucoside	I-3-Glucoside	Dp-3-Glucoside [M+6]		
7/27/2010	11.148	0.028	0.002	0.000	0.000	0.517	0.000	0.000	0.000
7/29/2010	8.179	0.000	0.000	0.000	0.000	0.298	0.000	0.000	0.000
7/30/2010	7.027	0.000	0.000	0.000	0.000	0.135	0.000	0.000	0.000
8/1/2010	4.701	0.000	0.000	0.000	0.000	0.196	0.000	0.000	0.000
8/5/2010	16.975	0.092	0.167	0.000	0.000	1.101	0.506	0.119	0.119
8/13/2010	42.989	1.635	1.751	0.019	0.019	5.832	5.827	0.191	0.191
8/17/2010	54.624	2.303	2.673	0.026	0.026	8.836	8.692	0.156	0.156
8/26/2010	61.163	3.174	2.857	0.034	0.034	18.035	9.492	0.239	0.239
9/9/2010	83.926	7.824	5.016	0.021	0.021	21.302	17.921	0.157	0.157
StErr	Q-3-Glucoside	L-3-Glucoside	K-3-Galactoside	K-3-Glucoside [M+6]	K-3-Glucoside	I-3-Glucoside	Dp-3-Glucoside [M+6]		
7/27/2010	3.218	0.008	0.001	0.000	0.000	0.149	0.000	0.000	0.000
7/29/2010	2.361	0.000	0.000	0.000	0.000	0.086	0.000	0.000	0.000
7/30/2010	2.028	0.000	0.000	0.000	0.000	0.039	0.000	0.000	0.000
8/1/2010	1.357	0.000	0.000	0.000	0.000	0.057	0.000	0.000	0.000
8/5/2010	4.900	0.027	0.048	0.000	0.000	0.318	0.146	0.034	0.034
8/13/2010	12.410	0.472	0.506	0.006	0.006	1.683	1.682	0.055	0.055
8/17/2010	15.769	0.665	0.772	0.008	0.008	2.551	2.509	0.045	0.045
8/26/2010	17.656	0.916	0.825	0.010	0.010	5.206	2.740	0.069	0.069
9/9/2010	24.227	2.258	1.448	0.006	0.006	6.149	5.173	0.045	0.045

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Supplementary Table 1

Mean values of

Sampling dates	Dp-3-Glucoside	Cn-3-Glucoside	Cn-3-Glucoside [M+6]	Pt-3-Glucoside [M+6]	Pt-3-Glucoside	Pn-3-Glucoside [M+6]
7/27/2010	0.000	0.000	0.000	0.000	0.000	0.000
7/29/2010	0.000	0.000	0.000	0.000	0.000	0.000
7/30/2010	0.000	0.000	0.000	0.000	0.000	0.000
8/1/2010	0.000	0.000	0.000	0.000	0.000	0.000
8/5/2010	19.523	10.188	0.113	0.170	14.274	0.235
8/13/2010	201.743	60.570	0.095	0.142	104.354	0.185
8/17/2010	277.855	67.778	0.095	0.231	155.007	0.285
8/26/2010	283.131	58.121	0.084	0.263	185.601	0.337
9/9/2010	251.693	43.137	0.048	0.214	164.439	0.353

Stdev	Dp-3-Glucoside	Cn-3-Glucoside	Cn-3-Glucoside [M+6]	Pt-3-Glucoside [M+6]	Pt-3-Glucoside	Pn-3-Glucoside [M+6]
7/27/2010	0.000	0.000	0.000	0.000	0.000	0.000
7/29/2010	0.000	0.000	0.000	0.000	0.000	0.000
7/30/2010	0.000	0.000	0.000	0.000	0.000	0.000
8/1/2010	0.000	0.000	0.000	0.000	0.000	0.000
8/5/2010	9.289	3.012	0.055	0.083	5.410	0.145
8/13/2010	120.654	31.119	0.048	0.061	59.523	0.068
8/17/2010	129.282	30.541	0.035	0.096	65.045	0.109
8/26/2010	65.474	22.275	0.057	0.153	17.739	0.173
9/9/2010	90.637	18.865	0.025	0.113	55.557	0.269

StErr	Dp-3-Glucoside	Cn-3-Glucoside	Cn-3-Glucoside [M+6]	Pt-3-Glucoside [M+6]	Pt-3-Glucoside	Pn-3-Glucoside [M+6]
7/27/2010	0.000	0.000	0.000	0.000	0.000	0.000
7/29/2010	0.000	0.000	0.000	0.000	0.000	0.000
7/30/2010	0.000	0.000	0.000	0.000	0.000	0.000
8/1/2010	0.000	0.000	0.000	0.000	0.000	0.000
8/5/2010	2.681	0.870	0.016	0.024	1.562	0.042
8/13/2010	34.830	8.983	0.014	0.018	17.183	0.020
8/17/2010	37.321	8.816	0.010	0.028	18.777	0.032
8/26/2010	18.901	6.430	0.017	0.044	5.121	0.050
9/9/2010	26.165	5.446	0.007	0.033	16.038	0.078

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Supplementary Table 1

Mean values of

Sampling dates	Pn-3-Glucoside	M-3-Glucoside [M+6]	M-3-Glucoside	Dp-3-Ac-Glucoside [M+6]	Dp-3-Ac-Glucoside	Cn-3-Ac-Glucoside [M+6]	
7/27/2010	0.000	0.000	0.000	0.000	0.000	0.000	0.000
7/29/2010	0.000	0.000	0.000	0.000	0.000	0.000	0.000
7/30/2010	0.000	0.000	0.000	0.000	0.000	0.000	0.000
8/1/2010	0.000	0.071	2.192	0.000	0.000	0.000	0.000
8/5/2010	15.429	0.520	35.592	0.096	10.848	0.033	0.033
8/13/2010	87.836	0.525	235.887	0.074	59.881	0.031	0.031
8/17/2010	119.554	1.058	489.617	0.105	78.771	0.032	0.032
8/26/2010	139.083	1.670	691.794	0.098	71.177	0.026	0.026
9/9/2010	124.094	2.234	780.271	0.091	62.939	0.016	0.016

Stdev	Pn-3-Glucoside	M-3-Glucoside [M+6]	M-3-Glucoside	Dp-3-Ac-Glucoside [M+6]	Dp-3-Ac-Glucoside	Cn-3-Ac-Glucoside [M+6]	
7/27/2010	0.000	0.000	0.000	0.000	0.000	0.000	0.000
7/29/2010	0.000	0.000	0.000	0.000	0.000	0.000	0.000
7/30/2010	0.000	0.000	0.000	0.000	0.000	0.000	0.000
8/1/2010	0.000	0.112	3.244	0.000	0.000	0.000	0.000
8/5/2010	5.869	0.306	17.070	0.046	3.447	0.046	0.046
8/13/2010	43.151	0.202	138.367	0.028	30.005	0.013	0.013
8/17/2010	46.181	0.472	92.530	0.041	33.166	0.012	0.012
8/26/2010	31.437	0.684	104.318	0.058	13.598	0.016	0.016
9/9/2010	42.459	1.368	220.134	0.056	17.754	0.008	0.008

StErr	Pn-3-Glucoside	M-3-Glucoside [M+6]	M-3-Glucoside	Dp-3-Ac-Glucoside [M+6]	Dp-3-Ac-Glucoside	Cn-3-Ac-Glucoside [M+6]	
7/27/2010	0.000	0.000	0.000	0.000	0.000	0.000	0.000
7/29/2010	0.000	0.000	0.000	0.000	0.000	0.000	0.000
7/30/2010	0.000	0.000	0.000	0.000	0.000	0.000	0.000
8/1/2010	0.000	0.032	0.936	0.000	0.000	0.000	0.000
8/5/2010	1.694	0.088	4.928	0.013	0.995	0.013	0.013
8/13/2010	12.457	0.058	39.943	0.008	8.662	0.004	0.004
8/17/2010	13.331	0.136	26.711	0.012	9.574	0.004	0.004
8/26/2010	9.075	0.197	30.114	0.017	3.925	0.005	0.005
9/9/2010	12.257	0.395	63.547	0.016	5.125	0.002	0.002

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Supplementary Table 1

Mean values of

Sampling dates	Cn-3-Ac-Glucoside	Pt-3-Ac-Glucoside [M+6]	Pt-3-Ac-Glucoside	Pn-3-Ac-Glucoside [M+6]	Pn-3-Ac-Glucoside	
7/27/2010	0.000	0.000	0.000	0.000	0.000	0.000
7/29/2010	0.000	0.000	0.000	0.000	0.000	0.000
7/30/2010	0.000	0.000	0.000	0.000	0.000	0.000
8/1/2010	0.000	0.000	0.000	0.000	0.000	0.000
8/5/2010	7.474	0.105	0.105	10.445	0.138	12.213
8/13/2010	19.062	0.072	0.072	47.069	0.080	35.293
8/17/2010	20.604	0.107	0.107	66.837	0.114	47.991
8/26/2010	17.400	0.109	0.109	68.327	0.119	52.680
9/9/2010	14.164	0.107	0.107	63.553	0.109	47.222

Stdev	Cn-3-Ac-Glucoside	Pt-3-Ac-Glucoside [M+6]	Pt-3-Ac-Glucoside	Pn-3-Ac-Glucoside [M+6]	Pn-3-Ac-Glucoside	
7/27/2010	0.000	0.000	0.000	0.000	0.000	0.000
7/29/2010	0.000	0.000	0.000	0.000	0.000	0.000
7/30/2010	0.000	0.000	0.000	0.000	0.000	0.000
8/1/2010	0.000	0.000	0.000	0.000	0.000	0.000
8/5/2010	0.834	0.049	0.049	3.154	0.074	4.688
8/13/2010	6.801	0.025	0.025	22.184	0.021	13.808
8/17/2010	6.789	0.040	0.040	24.397	0.040	15.595
8/26/2010	4.112	0.052	0.052	10.329	0.057	9.027
9/9/2010	3.542	0.064	0.064	16.520	0.067	11.110

StErr	Cn-3-Ac-Glucoside	Pt-3-Ac-Glucoside [M+6]	Pt-3-Ac-Glucoside	Pn-3-Ac-Glucoside [M+6]	Pn-3-Ac-Glucoside	
7/27/2010	0.000	0.000	0.000	0.000	0.000	0.000
7/29/2010	0.000	0.000	0.000	0.000	0.000	0.000
7/30/2010	0.000	0.000	0.000	0.000	0.000	0.000
8/1/2010	0.000	0.000	0.000	0.000	0.000	0.000
8/5/2010	0.241	0.014	0.014	0.910	0.021	1.353
8/13/2010	1.963	0.007	0.007	6.404	0.006	3.986
8/17/2010	1.960	0.011	0.011	7.043	0.012	4.502
8/26/2010	1.187	0.015	0.015	2.982	0.017	2.606
9/9/2010	1.022	0.018	0.018	4.769	0.019	3.207

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Mean values of

Sampling dates	M-3-Ac-Glucoside [M+6]	M-3-Ac-Glucoside	t-Pn-3-Cou-Glucoside [M+12]	t-Pn-3-Cou-Glucoside [M+6] Flav13	
7/27/2010	0.000	0.000	0.000	0.000	0.000
7/29/2010	0.000	0.000	0.000	0.000	0.000
7/30/2010	0.000	0.000	0.000	0.000	0.000
8/1/2010	0.000	0.000	0.000	0.000	0.000
8/5/2010	0.379	33.561	0.003	0.003	0.069
8/13/2010	0.327	127.638	0.001	0.001	0.040
8/17/2010	0.596	254.629	0.001	0.001	0.061
8/26/2010	0.841	352.516	0.001	0.001	0.064
9/9/2010	1.089	430.936	0.001	0.001	0.047
Stdev	M-3-Ac-Glucoside [M+6]	M-3-Ac-Glucoside	t-Pn-3-Cou-Glucoside [M+12]	t-Pn-3-Cou-Glucoside [M+6] Flav13	
7/27/2010	0.000	0.000	0.000	0.000	0.000
7/29/2010	0.000	0.000	0.000	0.000	0.000
7/30/2010	0.000	0.000	0.000	0.000	0.000
8/1/2010	0.000	0.000	0.000	0.000	0.000
8/5/2010	0.216	19.931	0.004	0.004	0.064
8/13/2010	0.106	62.783	0.000	0.000	0.012
8/17/2010	0.235	36.065	0.000	0.000	0.026
8/26/2010	0.254	66.216	0.001	0.001	0.021
9/9/2010	0.611	56.429	0.001	0.001	0.038
StErr	M-3-Ac-Glucoside [M+6]	M-3-Ac-Glucoside	t-Pn-3-Cou-Glucoside [M+12]	t-Pn-3-Cou-Glucoside [M+6] Flav13	
7/27/2010	0.000	0.000	0.000	0.000	0.000
7/29/2010	0.000	0.000	0.000	0.000	0.000
7/30/2010	0.000	0.000	0.000	0.000	0.000
8/1/2010	0.000	0.000	0.000	0.000	0.000
8/5/2010	0.062	5.754	0.001	0.001	0.018
8/13/2010	0.030	18.124	0.000	0.000	0.003
8/17/2010	0.068	10.411	0.000	0.000	0.008
8/26/2010	0.073	19.115	0.000	0.000	0.006
9/9/2010	0.176	16.290	0.000	0.000	0.011

Average, standard deviation, and standard error values for each timepoint in measured metabolites from the 2010 green berry incorporation trial

Supplementary Table 1

Mean values of

Sampling dates	t-Pn-3-Cou-Glucoside [M+6]	t-Pn-3-Cou-Glucoside	t-M-3-Cou-Glucoside [M+12]	t-M-3-Cou-Glucoside [M+6] Flav13	
7/27/2010	0.000	0.000	0.000	0.000	0.000
7/29/2010	0.000	0.000	0.000	0.000	0.000
7/30/2010	0.000	0.000	0.000	0.000	0.000
8/1/2010	0.000	0.000	0.000	0.000	0.000
8/5/2010	0.066	9.822	0.005	0.005	0.119
8/13/2010	0.039	21.342	0.002	0.002	0.073
8/17/2010	0.060	37.455	0.002	0.002	0.129
8/26/2010	0.068	38.680	0.004	0.004	0.211
9/9/2010	0.058	29.141	0.005	0.005	0.307

Stdev	t-Pn-3-Cou-Glucoside [M+6]	t-Pn-3-Cou-Glucoside	t-M-3-Cou-Glucoside [M+12]	t-M-3-Cou-Glucoside [M+6] Flav13	
7/27/2010	0.000	0.000	0.000	0.000	0.000
7/29/2010	0.000	0.000	0.000	0.000	0.000
7/30/2010	0.000	0.000	0.000	0.000	0.000
8/1/2010	0.000	0.000	0.000	0.000	0.000
8/5/2010	0.061	3.247	0.003	0.003	0.056
8/13/2010	0.012	9.059	0.001	0.001	0.030
8/17/2010	0.025	6.555	0.001	0.001	0.049
8/26/2010	0.023	3.201	0.002	0.002	0.062
9/9/2010	0.046	7.987	0.004	0.004	0.165

StErr	t-Pn-3-Cou-Glucoside [M+6]	t-Pn-3-Cou-Glucoside	t-M-3-Cou-Glucoside [M+12]	t-M-3-Cou-Glucoside [M+6] Flav13	
7/27/2010	0.000	0.000	0.000	0.000	0.000
7/29/2010	0.000	0.000	0.000	0.000	0.000
7/30/2010	0.000	0.000	0.000	0.000	0.000
8/1/2010	0.000	0.000	0.000	0.000	0.000
8/5/2010	0.018	0.937	0.001	0.001	0.016
8/13/2010	0.003	2.615	0.000	0.000	0.009
8/17/2010	0.007	1.892	0.000	0.000	0.014
8/26/2010	0.007	0.924	0.001	0.001	0.018
9/9/2010	0.013	2.306	0.001	0.001	0.048

Average, standard deviation, and standard error values for each timepoint in measured metabolites from the 2010 green berry incorporation trial

Supplementary Table 1

Mean values of

Sampling dates	t-M-3-Cou-Glucoside [M+6]	t-M-3-Cou-Glucoside
7/27/2010	0.000	0.000
7/29/2010	0.000	0.000
7/30/2010	0.000	0.000
8/1/2010	0.000	0.000
8/5/2010	0.116	10.354
8/13/2010	0.074	25.984
8/17/2010	0.132	53.470
8/26/2010	0.228	98.376
9/9/2010	0.350	115.619

Stdev	t-M-3-Cou-Glucoside [M+6]	t-M-3-Cou-Glucoside
7/27/2010	0.000	0.000
7/29/2010	0.000	0.000
7/30/2010	0.000	0.000
8/1/2010	0.000	0.000
8/5/2010	0.055	3.728
8/13/2010	0.030	13.044
8/17/2010	0.049	18.625
8/26/2010	0.069	20.760
9/9/2010	0.191	33.337

StErr	t-M-3-Cou-Glucoside [M+6]	t-M-3-Cou-Glucoside
7/27/2010	0.000	0.000
7/29/2010	0.000	0.000
7/30/2010	0.000	0.000
8/1/2010	0.000	0.000
8/5/2010	0.016	1.076
8/13/2010	0.009	3.766
8/17/2010	0.014	5.377
8/26/2010	0.020	5.993
9/9/2010	0.055	9.623