

Electronic supplementary information for:

**Kinetics of Hydrogen-Transfer Isomerizations of Butoxyl Radicals**

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Table S1. Cartesian coordinates (in Å) of all stationary points in reactions R1 – R5 by the M06-2X/MG3S method

Reactant of R1 and R2				Saddle point of R1			
C	-1.384361	0.403657	-0.009933	C	-5.367114	0.234242	-0.088521
C	-0.084521	-0.385233	-0.005979	C	-6.185702	1.505398	0.148489
C	1.138686	0.523850	0.006073	C	-5.826677	2.058401	1.529299
C	2.445775	-0.259679	0.000215	C	-4.337481	2.288630	1.610710
O	-2.527285	-0.343813	0.004909	O	-3.998798	0.485317	-0.017551
H	-1.447091	1.060205	0.877246	H	-3.887821	1.351722	0.908412
H	-1.432124	1.105553	-0.858653	H	-5.670752	-0.538389	0.629809
H	-0.075378	-1.042750	0.866209	H	-5.564235	-0.143066	-1.098589
H	-0.062431	-1.029494	-0.888118	H	-5.934964	2.236806	-0.622818
H	1.104962	1.188409	-0.861553	H	-7.250613	1.283450	0.072886
H	1.100983	1.169702	0.887687	H	-6.373073	2.987837	1.712670
H	3.310094	0.402925	0.009744	H	-6.140349	1.345165	2.293803
H	2.510880	-0.909978	0.873214	H	-3.883229	2.189033	2.592143
H	2.514911	-0.889633	-0.887294	H	-3.985985	3.170548	1.080264
Product of R1				Saddle point of R2			
C	-2.539074	-0.311085	-0.016676	C	-5.775837	1.551272	-0.213454
C	-1.291331	0.494328	0.018080	C	-6.147383	0.397444	-1.145686
C	-0.029100	-0.362267	-0.038224	C	-5.380131	0.776651	-2.413854
C	1.231609	0.472266	0.032994	C	-6.060892	1.758461	-3.331083
O	2.343353	-0.402242	-0.026131	O	-4.447082	1.875190	-0.563536
H	-2.546148	-1.320567	0.367977	H	-4.488687	1.394813	-1.783528
H	-3.485174	0.139753	-0.273567	H	-5.798530	1.277204	0.843451
H	1.240551	1.049487	0.964693	H	-6.438948	2.410078	-0.361893
H	-1.290064	1.213531	-0.806993	H	-5.763772	-0.539465	-0.744443
H	-1.262886	1.105881	0.932561	H	-7.221563	0.290692	-1.307052
H	-0.015175	-0.946442	-0.960201	H	-4.887133	-0.042658	-2.931493
H	-0.025964	-1.074131	0.790181	H	-6.431483	2.622010	-2.778248
H	1.252027	1.183276	-0.800865	H	-5.391594	2.113773	-4.112584
H	3.153383	0.107700	0.018221	H	-6.918670	1.282449	-3.815233

Product of R2

C	2.554658	-0.192996	0.079645
C	1.227796	0.461484	-0.060948
C	-0.014963	-0.353908	-0.103656
C	-1.266667	0.478862	0.092180
O	-2.386548	-0.380375	-0.013768
H	3.348348	0.528865	0.263857
H	2.551235	-0.915966	0.899176
H	2.827536	-0.753767	-0.824148
H	1.182157	1.489755	-0.397397
H	0.015931	-1.135567	0.661614
H	-0.107582	-0.882994	-1.063205
H	-1.235236	0.963211	1.073552
H	-1.305542	1.264667	-0.670466
H	-3.189403	0.124145	0.123833

Reactant of R3

C	1.814203	-0.568723	-0.011433
C	0.466940	0.095418	0.334967
C	-0.716039	-0.682522	-0.231134
C	-2.040925	0.003067	0.079543
O	0.559692	1.360342	-0.192012
H	2.641850	-0.004480	0.410776
H	1.817548	-1.577090	0.399161
H	1.931053	-0.622787	-1.092403
H	0.397180	0.156414	1.431428
H	-0.578249	-0.771131	-1.311146
H	-0.702373	-1.692502	0.185204
H	-2.881876	-0.547539	-0.338910
H	-2.194015	0.082550	1.156880
H	-2.053727	1.010392	-0.336558

Saddle point of R3

C	-5.848870	1.508756	-0.208303
C	-6.156914	0.361754	-1.170543
C	-5.344527	0.774454	-2.389234
C	-5.976095	1.177470	1.263811
O	-4.495581	1.830865	-0.495306
H	-4.479399	1.404135	-1.707307
H	-6.487684	2.367449	-0.451732
H	-5.761987	-0.567278	-0.756828
H	-7.221029	0.226763	-1.365921
H	-4.844047	0.001654	-2.962501
H	-5.796025	1.542698	-3.011720
H	-5.685218	2.027482	1.879034
H	-7.008934	0.918414	1.499814
H	-5.333578	0.332737	1.510722

Reactant of R4

C	0.859670	-0.694008	0.262983
C	-0.380182	0.016238	-0.353454
C	-0.477059	1.458479	0.126238
C	-1.625985	-0.782831	0.010490
O	1.967529	-0.015980	-0.148391
H	0.864852	-1.733904	-0.084507
H	0.746718	-0.655661	1.355250
H	-0.245060	0.002061	-1.436672
H	0.405132	2.031892	-0.150265
H	-1.354631	1.941867	-0.303550
H	-0.575413	1.489872	1.213404
H	-1.565552	-1.810806	-0.345772
H	-1.765679	-0.803133	1.092843
H	-2.509260	-0.321617	-0.431143

Saddle point of R4

C	-5.839013	1.525010	-0.225371
C	-6.168934	0.369380	-1.171974
C	-5.338456	0.773156	-2.386274
C	-7.648752	0.164314	-1.446311
O	-4.487947	1.834225	-0.495608
H	-4.462394	1.385979	-1.694751
H	-6.488474	2.384162	-0.435794
H	-5.737990	-0.541566	-0.752280
H	-4.864957	-0.007414	-2.973021
H	-5.782074	1.557459	-2.997654
H	-5.932938	1.263935	0.831043
H	-7.809645	-0.653532	-2.148799
H	-8.189221	-0.071562	-0.528540
H	-8.087077	1.067465	-1.874013

Product of R4

C	0.751270	-0.672635	0.245784
C	-0.449771	0.063099	-0.351327
C	-0.488939	1.472175	0.133191
C	-1.740327	-0.683734	0.016710
O	1.986455	-0.114553	-0.142250
H	1.968742	0.825208	0.059487
H	0.652494	-0.686301	1.339384
H	-0.332921	0.057678	-1.437188
H	-0.682939	2.301118	-0.529851
H	-0.502259	1.664186	1.199083
H	0.762294	-1.706656	-0.099054
H	-2.611691	-0.191677	-0.412172
H	-1.710390	-1.711399	-0.347999
H	-1.868370	-0.709159	1.100162

Saddle point of R5

C	-4.339616	1.909158	-0.514639
C	-5.788267	1.570016	-0.229661
C	-6.098327	0.365164	-1.141511
C	-5.397396	0.686484	-2.438947
O	-6.146247	1.589368	-3.185997
H	-3.598565	1.280783	-0.027777
H	-4.051284	2.952296	-0.569025
H	-4.415637	1.356862	-1.825250
H	-5.980517	1.346872	0.820377
H	-6.427507	2.406083	-0.511966
H	-5.656803	-0.540387	-0.721329
H	-7.165461	0.192284	-1.283743
H	-5.004341	-0.146471	-3.022035
H	-5.676659	1.815109	-3.990895

Product of R5

C	-2.472283	-0.260112	0.014331
C	-1.175748	0.533671	-0.085182
C	0.057802	-0.351905	0.063646
C	1.318359	0.424952	-0.008987
O	2.455000	-0.331451	-0.048767
H	-2.547401	-0.762796	0.979419
H	-3.344426	0.382699	-0.097640
H	-2.518084	-1.025586	-0.761352
H	-1.127747	1.052940	-1.044481
H	-1.157762	1.307406	0.686666
H	0.067207	-1.115804	-0.720049
H	-0.001728	-0.900749	1.015230
H	1.392428	1.399460	0.462747
H	3.228738	0.234401	-0.033253

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Table S2. Cartesian coordinates (in Å) of all stationary points in reactions R1 – R5 using the methods specified in Table 2 of text

Reactant of R1				Saddle point of R1			
C	2.453584	-0.258114	0.000032	C	-4.339934	2.300092	1.616229
C	1.140484	0.527360	0.009819	C	-5.831089	2.058431	1.534906
C	-0.083366	-0.391464	-0.008837	C	-6.185909	1.509209	0.144610
C	-1.389777	0.400158	-0.015693	C	-5.367228	0.230676	-0.087920
O	-2.534953	-0.340901	0.008370	O	-3.993906	0.484228	-0.013275
H	3.324350	0.407797	0.014584	H	-3.984604	3.182493	1.075580
H	2.517958	-0.918877	0.874435	H	-3.871109	2.188792	2.596796
H	-1.433173	1.117499	-0.862430	H	-5.564340	-0.156569	-1.101643
H	1.099355	1.172222	0.901328	H	-6.387657	2.989203	1.726546
H	1.104691	1.201696	-0.859693	H	-6.141638	1.332793	2.299912
H	-0.075640	-1.056118	0.867013	H	-5.922574	2.245750	-0.628363
H	-0.055445	-1.036893	-0.899004	H	-7.258721	1.292888	0.060118
H	-1.451529	1.059071	0.882192	H	-5.673835	-0.542772	0.639841
H	2.523507	-0.886828	-0.897321	H	-3.884248	1.339880	0.887671
Product of R1				Reactant of R2			
C	-2.548437	-0.308871	-0.00594	C	-1.395364	0.405457	-0.016088
C	-1.294775	0.497255	0.009746	C	-0.084949	-0.387905	-0.009377
C	-0.030635	-0.367305	-0.022777	C	1.146864	0.529057	0.010023
C	1.235107	0.474026	0.018532	C	2.462272	-0.261907	0.000088
O	2.351161	-0.400872	-0.014649	O	-2.543172	-0.346388	0.008243
H	-2.523530	-1.377605	0.19544	H	1.115300	1.206286	-0.862920
H	-3.517305	0.161284	-0.152097	H	-1.465454	1.057936	0.889948
H	-1.287123	1.199782	-0.841629	H	-1.445270	1.124983	-0.864559
H	-1.268552	1.141029	0.910393	H	-0.080458	-1.055903	0.869381
H	-0.018600	-0.984307	-0.932081	H	-0.059436	-1.035591	-0.903317
H	-0.025530	-1.057262	0.833249	H	1.109585	1.175669	0.905812
H	1.243773	1.086009	0.936874	H	3.336399	0.406941	0.015330
H	1.251187	1.162756	-0.84365	H	2.527820	-0.925291	0.877828
H	3.168835	0.104660	0.013333	H	2.533946	-0.892138	-0.901322

Saddle point of R2

C	-5.773976	1.552615	-0.203160
C	-6.151304	0.391065	-1.141709
C	-5.382449	0.770262	-2.420218
C	-6.064305	1.760746	-3.343770
O	-4.437355	1.877613	-0.562429
H	-4.476484	1.406463	-1.766993
H	-5.790671	1.277404	0.865037
H	-6.443356	2.421552	-0.350645
H	-5.766209	-0.558040	-0.738046
H	-7.237663	0.284800	-1.303642
H	-4.872496	-0.053618	-2.939511
H	-6.438265	2.634449	-2.785788
H	-5.386033	2.120186	-4.131735
H	-6.931138	1.282416	-3.836026

Product of R2

C	-1.275315	0.482655	0.099428
C	-0.017550	-0.358744	-0.112169
C	1.237124	0.459725	-0.084977
C	2.573242	-0.192438	0.088453
O	-2.400965	-0.380116	-0.012798
H	-3.216079	0.117499	0.133196
H	-1.241041	0.960426	1.096473
H	-1.317363	1.284139	-0.663353
H	0.017788	-1.148635	0.661239
H	-0.127551	-0.893013	-1.080138
H	1.188199	1.512257	-0.386286
H	2.855648	-0.793697	-0.800017
H	3.373452	0.544669	0.251341
H	2.569655	-0.889901	0.945524

Reactant of R3

C	0.468855	0.097920	0.338919
C	-0.722572	-0.689742	-0.226923
C	-2.056187	0.005755	0.076731
C	1.827956	-0.571944	-0.014456
O	0.565577	1.367016	-0.193617
H	-2.066204	1.019286	-0.354679
H	0.409203	0.164155	1.447651
H	-0.581101	-0.787364	-1.317572
H	-0.710663	-1.707658	0.201520
H	-2.905650	-0.553818	-0.343137
H	-2.215337	0.097287	1.164034
H	2.665184	-0.000239	0.407870
H	1.829932	-1.589700	0.404466
H	1.941713	-0.630020	-1.106837

Saddle point of R3

C	-5.855334	1.515803	-0.206623
C	-6.165171	0.360456	-1.177294
C	-5.342932	0.768083	-2.402716
C	-5.973697	1.176187	1.276000
O	-4.492913	1.841069	-0.499274
H	-4.470682	1.421358	-1.698387
H	-6.500514	2.384821	-0.447738
H	-5.773140	-0.580688	-0.756605
H	-7.240373	0.227931	-1.380126
H	-4.821284	-0.013766	-2.967164
H	-5.793486	1.537654	-3.044432
H	-5.672506	2.031936	1.898369
H	-7.015515	0.914987	1.523371
H	-5.322340	0.321523	1.516603

Product of R3

C	-0.428955	0.037340	-0.340629
C	0.790368	-0.700337	0.230947
C	2.084878	-0.034749	-0.114105
C	-1.740796	-0.671202	0.007029
O	-0.393990	1.352508	0.216554
H	-1.119588	1.880066	-0.144386
H	-0.317227	0.101271	-1.441350
H	0.652643	-0.742204	1.333365
H	0.777241	-1.744886	-0.126086
H	3.010531	-0.607811	-0.193254
H	2.135913	1.055467	-0.150535
H	-2.607967	-0.120029	-0.393058
H	-1.762225	-1.687599	-0.417772
H	-1.850369	-0.740653	1.101186

Reactant of R4

C	0.866709	-0.690401	0.267803
C	-0.381340	0.018515	-0.360180
C	-0.484995	1.462722	0.127413
C	-1.624531	-0.792485	0.009618
O	1.970850	-0.016358	-0.152778
H	0.405349	2.040859	-0.137549
H	0.744435	-0.620495	1.365659
H	-0.242724	0.003672	-1.448942
H	-1.364555	1.950150	-0.310452
H	-0.595545	1.485230	1.220412
H	0.864422	-1.745999	-0.054779
H	-1.555894	-1.826906	-0.346445
H	-1.759668	-0.810217	1.099316
H	-2.517680	-0.335537	-0.432911

Saddle point of R4

C	-5.836338	1.525660	-0.223457
C	-6.167010	0.363280	-1.172293
C	-5.340233	0.768336	-2.393833
C	-7.654270	0.162809	-1.445932
O	-4.482079	1.839201	-0.496791
H	-4.453553	1.399477	-1.682091
H	-6.493457	2.387375	-0.436960
H	-5.733815	-0.553303	-0.750389
H	-4.852001	-0.011021	-2.980870
H	-5.784762	1.559387	-3.006780
H	-5.930876	1.265407	0.839581
H	-7.821559	-0.658562	-2.152635
H	-8.197791	-0.071677	-0.522044
H	-8.090128	1.074642	-1.874852

Product of R4

C	0.743130	-0.692761	0.236047
C	-0.452649	0.064754	-0.357026
C	-0.455822	1.476516	0.135121
C	-1.757328	-0.663205	0.025568
O	1.982646	-0.124174	-0.136649
H	1.934489	0.826658	0.023607
H	0.635871	-0.719725	1.335949
H	-0.346551	0.058416	-1.450765
H	-0.696916	2.315222	-0.511035
H	-0.353268	1.670111	1.203262
H	0.750215	-1.728617	-0.123956
H	-2.630474	-0.159913	-0.402544
H	-1.741462	-1.699263	-0.336171
H	-1.877051	-0.681325	1.116588

Reactant of R5

C	-2.557026	-0.313191	-0.009932
C	-1.300515	0.500118	0.017653
C	-0.029119	-0.363420	-0.036732
C	1.242042	0.477066	0.030146
O	2.356266	-0.406133	-0.023109
H	-2.554335	-1.352549	0.328962
H	-3.517205	0.138196	-0.267747
H	1.252861	1.065514	0.968298
H	-1.301221	1.221371	-0.821709
H	-1.271867	1.123945	0.937907
H	-0.013746	-0.957636	-0.965885
H	-0.022709	-1.078835	0.803864
H	1.265288	1.188991	-0.817793
H	3.180509	0.096636	0.012170

Saddle point of R5

C	-4.333932	1.913089	-0.516200
C	-5.791868	1.571722	-0.226769
C	-6.103318	0.354428	-1.139207
C	-5.397083	0.674431	-2.445574
O	-6.145695	1.594598	-3.186897
H	-3.582631	1.288595	-0.013206
H	-4.044830	2.967879	-0.583647
H	-4.400525	1.353074	-1.820744
H	-5.984757	1.351560	0.836172
H	-6.439426	2.414433	-0.516782
H	-5.658687	-0.560516	-0.711161
H	-7.181903	0.180199	-1.284269
H	-5.009891	-0.166319	-3.043053
H	-5.672080	1.846449	-3.991061

Product of R5

C	-2.488954	-0.262511	0.015435
C	-1.184577	0.538811	-0.089400
C	0.058067	-0.353950	0.062779
C	1.328981	0.427000	0.001296
O	2.470854	-0.333542	-0.047752
H	-2.564590	-0.766583	0.992983
H	-3.371690	0.385120	-0.099709
H	-2.536259	-1.039560	-0.765159
H	-1.138528	1.060060	-1.061016
H	-1.167465	1.323358	0.688567
H	0.071775	-1.121809	-0.733041
H	-0.008592	-0.913699	1.021426
H	1.410211	1.417394	0.465756
H	3.257203	0.227960	-0.068460

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Table S3. Rate constants (in s<sup>-1</sup>) of reactions R1 – R5

T(K)	TST	CVT	CVT/ZCT	CVT/SCT
R1: M08-SO/MG3S (harmonic-oscillator approximation for vibrations)				
200	5.32E+00	4.44E+00	5.65E+02	7.38E+04
250	8.63E+02	7.40E+02	1.01E+04	2.31E+05
298	2.24E+04	1.95E+04	1.07E+05	8.47E+05
300	2.51E+04	2.19E+04	1.17E+05	8.95E+05
350	2.76E+05	2.43E+05	7.92E+05	3.33E+06
400	1.67E+06	1.48E+06	3.57E+06	1.05E+07
500	2.06E+07	1.84E+07	3.19E+07	6.37E+07
600	1.12E+08	9.99E+07	1.45E+08	2.36E+08
700	3.76E+08	3.37E+08	4.42E+08	6.32E+08
800	9.44E+08	8.45E+08	1.04E+09	1.37E+09
900	1.95E+09	1.74E+09	2.04E+09	2.54E+09
1000	3.49E+09	3.11E+09	3.53E+09	4.22E+09
1500	2.10E+10	1.85E+10	1.94E+10	2.10E+10
2000	5.30E+10	4.61E+10	4.73E+10	4.94E+10
2400	8.49E+10	7.34E+10	7.45E+10	7.68E+10
2500	9.34E+10	8.06E+10	8.16E+10	8.40E+10
R2: M08-SO/6-31+G(d,p) (harmonic-oscillator approximation for vibrations)				
200	8.37E-09	8.37E-09	3.36E-05	1.89E-02
250	9.49E-05	9.48E-05	6.63E-03	3.42E-01
298	3.85E-02	3.84E-02	5.40E-01	5.64E+00
300	4.75E-02	4.73E-02	6.36E-01	6.33E+00
350	4.00E+00	3.98E+00	2.35E+01	9.87E+01
400	1.11E+02	1.11E+02	4.03E+02	1.08E+03
500	1.17E+04	1.16E+04	2.53E+04	4.40E+04
600	2.64E+05	2.60E+05	4.37E+05	6.26E+05
700	2.46E+06	2.41E+06	3.48E+06	4.49E+06
800	1.32E+07	1.29E+07	1.69E+07	2.04E+07
900	4.89E+07	4.78E+07	5.87E+07	6.79E+07
1000	1.40E+08	1.37E+08	1.60E+08	1.80E+08
1500	3.42E+09	3.27E+09	3.42E+09	3.60E+09
2000	1.73E+10	1.63E+10	1.63E+10	1.68E+10
2400	3.91E+10	3.66E+10	3.59E+10	3.66E+10
2500	4.61E+10	4.30E+10	4.20E+10	4.28E+10

R3: M08-SO/6-31+G(d,p) (harmonic-oscillator approximation for vibrations)

200	3.99E-10	3.37E-10	4.55E-05	6.49E-02
250	9.11E-06	7.90E-06	4.71E-03	5.51E-01
298	5.84E-03	5.16E-03	2.59E-01	5.47E+00
300	7.31E-03	6.46E-03	3.02E-01	6.02E+00
350	8.70E-01	7.77E-01	9.92E+00	6.57E+01
400	3.14E+01	2.83E+01	1.74E+02	6.11E+02
500	4.83E+03	4.39E+03	1.28E+04	2.46E+04
600	1.40E+05	1.28E+05	2.61E+05	3.90E+05
700	1.58E+06	1.44E+06	2.39E+06	3.15E+06
800	9.77E+06	8.92E+06	1.30E+07	1.59E+07
900	4.07E+07	3.71E+07	4.98E+07	5.80E+07
1000	1.28E+08	1.17E+08	1.47E+08	1.66E+08
1500	4.16E+09	3.74E+09	4.08E+09	4.29E+09
2000	2.45E+10	2.16E+10	2.24E+10	2.30E+10
2400	5.99E+10	5.23E+10	5.29E+10	5.39E+10
2500	7.18E+10	6.25E+10	6.28E+10	6.40E+10

R4: M08-SO/cc-pVTZ+ (harmonic-oscillator approximation for vibrations)

200	1.77E-10	1.46E-10	5.79E-05	5.07E-02
250	4.81E-06	4.09E-06	6.06E-03	5.98E-01
298	3.44E-03	2.98E-03	2.88E-01	6.48E+00
300	4.33E-03	3.75E-03	3.33E-01	7.14E+00
350	5.58E-01	4.93E-01	9.80E+00	7.51E+01
400	2.14E+01	1.90E+01	1.60E+02	6.42E+02
500	3.56E+03	3.18E+03	1.11E+04	2.31E+04
600	1.09E+05	9.76E+04	2.23E+05	3.50E+05
700	1.27E+06	1.13E+06	2.04E+06	2.77E+06
800	8.06E+06	7.20E+06	1.12E+07	1.39E+07
900	3.42E+07	3.04E+07	4.27E+07	5.05E+07
1000	1.09E+08	9.70E+07	1.26E+08	1.45E+08
1500	3.72E+09	3.22E+09	3.55E+09	3.75E+09
2000	2.23E+10	1.90E+10	1.96E+10	2.02E+10
2400	5.52E+10	4.62E+10	4.65E+10	4.75E+10
2500	6.62E+10	5.52E+10	5.53E+10	5.64E+10

R5: M08-SO/6-31+G(d,p) (hindered-rotor approximation for selected torsion modes (see the text in the article for the specification of these torsions modes) and harmonic-oscillator approximation for the other vibrational modes)

200	5.73E-13	5.66E-13	4.02E-07	1.69E-04
250	2.61E-08	2.58E-08	6.79E-05	2.85E-03
298	2.62E-05	2.59E-05	4.24E-03	4.51E-02
300	3.33E-05	3.30E-05	4.95E-03	5.04E-02
350	5.54E-03	5.49E-03	1.67E-01	7.13E-01
400	2.59E-01	2.57E-01	3.01E+00	7.63E+00
500	5.79E+01	5.75E+01	2.47E+02	3.79E+02
600	2.20E+03	2.19E+03	5.76E+03	7.29E+03
700	3.05E+04	3.03E+04	6.04E+04	7.01E+04
800	2.23E+05	2.22E+05	3.73E+05	4.13E+05
900	1.07E+06	1.06E+06	1.59E+06	1.72E+06
1000	3.79E+06	3.77E+06	5.22E+06	5.53E+06
1500	1.88E+08	1.87E+08	2.15E+08	2.20E+08
2000	1.45E+09	1.44E+09	1.55E+09	1.57E+09
2400	4.16E+09	4.12E+09	4.34E+09	4.38E+09
2500	5.15E+09	5.10E+09	5.35E+09	5.39E+09

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