

Electronic supplementary information (ESI)

Theoretical and experimental mechanistic study of water molecule involvement in the Prilezhaev reaction

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Cartesian coordinates of all structures calculated at the B3PW91 functional

Reactant(1mCPBA)	2
TS(1mCPBA)	2
Product(1mCPBA)	2
Reactant(2mCPBA)	2
TS(2mCPBA)	3
Product(2mCPBA)	3
Reactant(1W)	4
TS(1W)	4
Product(1W)	4
Reactant(2W)	5
TS(2W)	5
Product(2W)	6

Reactant(1mCPBA)

C	0.28728600	1.98960300	3.94068500
H	1.36842300	2.06919400	3.96640600
H	-0.26812700	2.91683500	4.03763100
C	-0.30587600	0.79847200	3.80784300
H	0.33025100	-0.08075300	3.72303400
O	0.23742500	2.51378600	0.71172700
H	0.31730900	1.70150200	1.26299300
O	0.46851900	2.01671200	-0.59914500
C	0.76324000	0.70172300	-0.59514400
O	0.80163600	0.05857700	0.42846200
C	1.01606600	0.18795100	-1.96171500
C	0.98896100	1.01012800	-3.09060100
C	1.23639600	0.45940300	-4.34100600
C	1.50852500	-0.89825100	-4.47625500
C	1.53187600	-1.70339900	-3.34174400
C	1.28923000	-1.17556900	-2.08303800
H	0.77713000	2.06690800	-2.98766000
H	1.21825800	1.08995500	-5.22309100
H	1.70165400	-1.33202800	-5.45029000
Cl	1.87221400	-3.40464400	-3.50567600
H	1.30709400	-1.79987100	-1.19838200
C	-1.74618200	0.51518200	3.76884300
C	-2.16730300	-0.81847100	3.69451300
C	-2.72733400	1.51626900	3.80943500
C	-3.51813500	-1.14639800	3.66819400
H	-1.42051100	-1.60614200	3.65680900
C	-4.07559700	1.19118800	3.78111800
H	-2.43488100	2.55974400	3.85766800
C	-4.47846900	-0.14184200	3.71201400
H	-3.81996200	-2.18724200	3.61172300
H	-4.81921500	1.98112500	3.81130800
H	-5.53399900	-0.39229300	3.69019700

TS(1mCPBA)

C	-2.80130700	-0.37698900	2.31512000
H	-2.26866900	-0.93542100	3.07477700
H	-3.14362500	0.60818000	2.60327300
C	-3.30071700	-1.02407600	1.21658000
H	-3.00088800	-2.05966000	1.06672100
O	-1.29076400	0.24347300	1.23696500
H	-0.83212100	-0.63214200	1.13356000
O	0.24489700	1.00853500	0.76653300
C	1.07340000	0.02710200	0.58737600
O	0.77400500	-1.15902400	0.73213900
C	2.45311100	0.44864600	0.17917700
C	2.79157000	1.79174200	0.01177100
C	4.08322300	2.13214100	-0.37044600
C	5.04020300	1.14543200	-0.58624100
C	4.68621000	-0.18867900	-0.41419000
C	3.40277000	-0.55064300	-0.03415300
H	2.04180100	2.55489100	0.18099600
H	4.35347600	3.17431300	-0.50313700

H	6.04956000	1.40339600	-0.88442600
Cl	5.88360200	-1.43193100	-0.68252500
H	3.12345500	-1.58825400	0.09945800
C	-4.18248100	-0.47949600	0.20241500
C	-4.64336100	-1.33047300	-0.81492400
C	-4.60547300	0.86035900	0.19654400
C	-5.50830100	-0.86658300	-1.79633900
H	-4.31592300	-2.36577500	-0.82774400
C	-5.46416900	1.32306100	-0.78665300
H	-4.24413500	1.54583100	0.95447600
C	-5.92171800	0.46200400	-1.78465400
H	-5.85588400	-1.53916400	-2.57321600
H	-5.77711400	2.36181900	-0.78245100
H	-6.59402700	0.82965400	-2.55276300

Product(1mCPBA)

C	-1.42394100	2.41482800	1.78446400
H	-0.55306000	2.84532900	1.29790200
H	-2.15385700	3.10417300	2.20019300
C	-1.32183100	1.06142200	2.34767600
H	-0.36110900	0.56743200	2.21968200
O	-2.00255100	1.29498800	1.09789000
H	-1.23830700	0.74623600	-0.33290500
O	1.04095100	0.97667600	-0.00093700
C	0.52028400	0.54658000	-1.01042700
O	-0.79620300	0.42960500	-1.16213800
C	1.29577800	0.09867400	-2.20220700
C	2.68801300	0.17713900	-2.15666300
C	3.43909100	-0.23227100	-3.24999800
C	2.81224800	-0.72110900	-4.39252300
C	1.42380000	-0.79368400	-4.42444800
C	0.65496000	-0.38958200	-3.34243700
H	3.15895900	0.56026700	-1.25908100
H	4.52178300	-0.17362300	-3.21991700
H	3.39015200	-1.04327000	-5.25074400
Cl	0.63249700	-1.40586500	-5.85534100
H	-0.42487100	-0.45028000	-3.37738100
C	-2.15013500	0.60230500	3.49200600
C	-1.52183600	0.03209000	4.60035800
C	-3.53909900	0.74148500	3.49012300
C	-2.26880900	-0.37556400	5.70057700
H	-0.44288800	-0.09356400	4.60155600
C	-4.28468600	0.32773400	4.58801200
H	-4.03045200	1.15626600	2.61635000
C	-3.65235400	-0.22767200	5.69737800
H	-1.76994600	-0.81608100	6.55757700
H	-5.36466100	0.43329100	4.57526200
H	-4.23673800	-0.55114400	6.55241200

Reactant(2mCPBA)

C	-3.56232800	1.21828800	2.42246700
H	-2.57241000	1.65761100	2.46735300
H	-4.15145600	1.44959900	1.54090000

C	-4.01128100	0.43487100	3.40613800
H	-3.35704300	0.25867200	4.25863200
O	-1.34158000	1.12004200	-1.26310900
O	-0.66359900	0.85151200	-2.48149600
C	0.45768300	1.58097100	-2.62839900
O	0.94906800	2.26998100	-1.76193000
C	1.03024700	1.41093300	-3.98780100
C	0.38128800	0.68774600	-4.99169300
C	0.97253900	0.57756400	-6.24347000
C	2.20010400	1.17833800	-6.50264700
C	2.83328700	1.89618300	-5.49256700
C	2.26182300	2.02043100	-4.23597700
H	-0.57538900	0.22197000	-4.79268700
H	0.47540800	0.01957000	-7.02923500
H	2.66485400	1.09474100	-7.47801100
Cl	4.37043700	2.65153600	-5.81260700
H	2.75110800	2.58206500	-3.45005200
C	-5.31602200	-0.23374700	3.49069800
C	-5.63668300	-0.94965600	4.65127100
C	-6.26613800	-0.19382900	2.45977000
C	-6.85977200	-1.59765500	4.78526000
H	-4.91257400	-0.99443100	5.45990100
C	-7.48707900	-0.83928300	2.59125800
H	-6.04674500	0.34372800	1.54350000
C	-7.79184600	-1.54446900	3.75488100
H	-7.08384400	-2.14463300	5.69549100
H	-8.20717200	-0.79591500	1.78021800
H	-8.74735500	-2.04906200	3.85359600
H	-0.81567200	0.60182200	-0.60589500
O	0.37208800	2.30434800	0.91121000
H	0.53354800	2.38595000	-0.06083100
O	1.45210300	1.48771600	1.33897400
C	1.26537300	0.18359000	1.06088000
O	0.36785500	-0.25157500	0.37458000
C	2.32114100	-0.65153800	1.68765200
C	3.30413300	-0.11768100	2.52482100
C	2.29254600	-2.01967800	1.40990700
C	4.25774100	-0.96070400	3.08021700
H	3.31746000	0.94344200	2.73847200
C	3.25416200	-2.84186300	1.97588400
H	1.52193600	-2.41995600	0.76300900
C	4.24071700	-2.32522600	2.81038900
H	5.02395000	-0.55562900	3.73198500
H	4.98287700	-2.98624600	3.24235100
Cl	3.22734100	-4.55051200	1.63676800

TS(2mCPBA)

C	-3.64027000	1.53610500	5.00944300
H	-2.71356200	1.98180000	5.34817400
H	-4.30522900	2.17001300	4.43683100
C	-4.05168100	0.34155800	5.52823300
H	-3.35234000	-0.18974400	6.17023100
O	-2.90218500	0.54000500	3.42478000
O	-2.25073200	0.10110500	1.86036400
C	-1.32228000	0.89881600	1.44493100
O	-0.69746400	1.72615800	2.10879700

C	-1.01725000	0.72201100	-0.01787700
C	-1.80530600	-0.08177100	-0.84257500
C	-1.48618100	-0.20634400	-2.18918400
C	-0.38557900	0.45881600	-2.72006200
C	0.39091000	1.25433800	-1.88392500
C	0.08851200	1.39540300	-0.53816100
H	-2.66007500	-0.59771800	-0.42324800
H	-2.09698600	-0.82655900	-2.83649700
H	-0.12987200	0.36519400	-3.76897100
Cl	1.77355300	2.09285700	-2.54421600
H	0.68749900	2.01992500	0.11260800
C	-5.32064000	-0.32505000	5.30180500
C	-5.57636800	-1.53062700	5.97435500
C	-6.30967100	0.18305200	4.44305600
C	-6.78062500	-2.20060900	5.80768100
H	-4.81669300	-1.93851500	6.63443300
C	-7.50903300	-0.48896600	4.27346500
H	-6.13119800	1.10092700	3.89466900
C	-7.75103700	-1.68135600	4.95619700
H	-6.96123300	-3.12951500	6.33816800
H	-8.26125200	-0.08673700	3.60300000
H	-8.69222300	-2.20378500	4.82018800
H	-2.15124800	0.13885900	3.92177200
O	-0.38622400	2.02052100	4.68096600
H	-0.53500800	1.92723000	3.69123600
O	0.72700900	1.17142700	4.91108000
C	0.38010900	-0.12067700	5.04677000
O	-0.73221800	-0.56069900	4.86365600
C	1.55368700	-0.94475800	5.44097400
C	2.78810900	-0.38395000	5.77740100
C	1.37350900	-2.32881900	5.46995300
C	3.83886500	-1.21551500	6.14272800
H	2.91922500	0.69035200	5.75460400
C	2.43645100	-3.13918000	5.83673800
H	0.41122900	-2.74956000	5.20622000
C	3.67217000	-2.59618000	6.17461700
H	4.79999600	-0.78835500	6.40698000
H	4.48954700	-3.24870900	6.45812500
Cl	2.22109500	-4.86869400	5.87510200

Product(2mCPBA)

C	-2.68872600	1.61374400	1.90701800
H	-1.64836400	1.80549400	2.15156000
H	-3.43216700	2.31702800	2.27341700
C	-3.10841100	0.23427200	1.62063300
H	-2.32417300	-0.51697200	1.66721000
O	-2.92100300	1.18586700	0.55350900
O	-1.56389000	0.75842100	-1.68991400
C	-0.42392000	1.36435800	-1.95145600
O	0.17587400	2.07804200	-1.16181000
C	0.08614200	1.10620100	-3.32556900
C	-0.60715400	0.29512700	-4.22567800
C	-0.09085800	0.08558900	-5.49837000
C	1.10787100	0.67837600	-5.88143400
C	1.78694700	1.48525300	-4.97341500

C	1.29018400	1.70589500	-3.69861700
H	-1.54049700	-0.16273800	-3.92328600
H	-0.62311100	-0.54387000	-6.20322800
H	1.51534700	0.51948400	-6.87293600
Cl	3.29037200	2.23117100	-5.44956400
H	1.81581900	2.33417800	-2.99043900
C	-4.49377400	-0.24880100	1.85426800
C	-4.69382500	-1.39923100	2.61906700
C	-5.60001600	0.43113400	1.34184700
C	-5.98151100	-1.85278500	2.88540500
H	-3.83707300	-1.94098800	3.00940600
C	-6.88611800	-0.02699800	1.60357700
H	-5.44373400	1.30919900	0.72411000
C	-7.08127300	-1.16714400	2.37880700
H	-6.12514300	-2.74668700	3.48357100
H	-7.73980200	0.50495100	1.19609800
H	-8.08600600	-1.52333100	2.58108400
H	-1.91130600	0.97644800	-0.78370200
O	0.57434400	2.38601600	1.48541900
H	0.40343300	2.30023000	0.51554400
O	1.70244600	1.54310200	1.66260000
C	1.35671900	0.26768800	1.97015700
O	0.23071500	-0.15221800	1.98974900
C	2.57807200	-0.53509400	2.26667600
C	3.86317700	0.01216600	2.27627800
C	2.38658800	-1.88995300	2.54243300
C	4.95160200	-0.80218800	2.56279100
H	4.00567100	1.06384600	2.06335700
C	3.48671700	-2.68371200	2.82631700
H	1.38473000	-2.30073000	2.53239500
C	4.77296300	-2.15365900	2.83904700
H	5.95221400	-0.38400700	2.57266700
H	5.61893400	-2.79265400	3.06316900
Cl	3.25453800	-4.37726900	3.17287300

Reactant(1W)

C	4.06078500	1.11951300	1.51403600
H	3.41724700	1.90739300	1.88805400
H	3.67946700	0.10728700	1.60023400
C	5.24882300	1.40474800	0.97449000
H	5.54757300	2.45140400	0.92153300
O	-0.38472800	0.07962500	0.84367900
O	-1.62846800	-0.51809800	0.50335300
C	-2.58332700	0.36184900	0.13227900
O	-2.38273200	1.52473300	-0.12615700
C	-3.90699600	-0.31183800	0.04780100
C	-4.11766300	-1.61956800	0.49174800
C	-5.38519800	-2.17876000	0.39179800
C	-6.44112900	-1.45055200	-0.14662700
C	-6.21552700	-0.14889600	-0.58362500
C	-4.95941300	0.43016800	-0.49188900
H	-3.29809000	-2.18595600	0.91510000
H	-5.55824700	-3.19208700	0.73733600
H	-7.43159000	-1.88303700	-0.22618000
Cl	-7.53491300	0.76950700	-1.25752500
H	-4.78369800	1.44572500	-0.82448700

C	6.22787900	0.46011400	0.42055200
C	7.40278500	0.96275600	-0.15312100
C	6.04613600	-0.93072000	0.43558600
C	8.36112600	0.11402000	-0.69653200
H	7.56265700	2.03708500	-0.17240800
C	7.00121300	-1.77918500	-0.10530900
H	5.15023500	-1.35383800	0.87773100
C	8.16411000	-1.26204600	-0.67535900
H	9.26268000	0.52902200	-1.13575900
H	6.84057800	-2.85241900	-0.08208100
H	8.90918800	-1.92883300	-1.09681100
H	-0.10073000	0.54840700	0.01894100
H	0.30018200	1.58405400	-2.16818600
O	0.18605600	1.72784500	-1.22569900
H	-0.70018500	2.09767800	-1.10235600

TS(1W)

C	2.56424300	1.34100300	1.56444200
H	2.02408600	2.25365500	1.78046600
H	2.53049100	0.57004800	2.32335500
C	3.47871500	1.31788600	0.54875400
H	3.51444000	2.18747500	-0.10368500
O	1.22535800	0.49875600	0.36560700
O	-0.25525300	-0.27166100	-0.17382400
C	-1.31831000	0.45151800	0.00417300
O	-1.36360000	1.66462800	0.19344900
C	-2.58451200	-0.36010800	-0.07013700
C	-2.56707600	-1.75441200	-0.12455600
C	-3.76506800	-2.45579500	-0.18635200
C	-4.98103200	-1.77990000	-0.19881400
C	-4.98117600	-0.38990800	-0.14547700
C	-3.79755600	0.32925800	-0.08094200
H	-1.61739500	-2.27459900	-0.11499200
H	-3.75799900	-3.53991200	-0.22520000
H	-5.91915300	-2.32006800	-0.24796700
Cl	-6.50444500	0.46559500	-0.15914600
H	-3.79571700	1.41088800	-0.03161700
C	4.40291500	0.24718200	0.22430500
C	5.32956400	0.44888300	-0.81111300
C	4.42070300	-0.98181400	0.90506800
C	6.25194300	-0.53272100	-1.14696600
H	5.32213000	1.39157500	-1.35023400
C	5.33755400	-1.96291500	0.56493000
H	3.70104000	-1.17474200	1.69239200
C	6.25867800	-1.74254700	-0.45948600
H	6.96257900	-0.35636400	-1.94749200
H	5.33497100	-2.90900200	1.09606200
H	6.97490600	-2.51424900	-0.72153400
H	1.15666600	1.28254500	-0.23444200
H	0.62106500	3.15380800	-1.74148000
O	0.77491800	2.93615200	-0.81915100
H	-0.10468000	2.70600900	-0.44517600

Product(1W)

C	3.34339400	0.51212000	1.74661000	C1	4.65593400	3.80544100	-3.61483600
H	2.57463400	1.18433200	2.12042100	H	2.97189000	2.18168400	-1.96119800
H	3.83857900	-0.11249300	2.48567700	C	-4.24889900	-0.64396100	4.55881500
C	4.06005400	0.84015300	0.50426500	C	-4.41712900	-1.08902000	5.87637300
H	3.76671900	1.75729200	-0.00378800	C	-5.33520800	-0.01233100	3.93569500
O	3.02523600	-0.15618200	0.52281500	C	-5.62051900	-0.91207700	6.55044200
O	-1.71677800	-0.87448800	-1.48146100	H	-3.58807900	-1.58215200	6.37610800
C	-2.32981300	-0.23720600	-0.64462900	C	-6.53665600	0.16561400	4.60592300
O	-1.77204700	0.68376500	0.13194000	H	-5.23991600	0.34274000	2.91514800
C	-3.78837800	-0.42367300	-0.39830500	C	-6.68687000	-0.28315000	5.91753800
C	-4.47614900	-1.37140900	-1.15661300	H	-5.72467800	-1.26665200	7.57092800
C	-5.83510300	-1.56689800	-0.95086000	H	-7.36405000	0.65678300	4.10352100
C	-6.51733600	-0.82364100	0.00799400	H	-7.62818100	-0.14294400	6.43872100
C	-5.81908200	0.11766900	0.75653600	H	2.63541600	-3.20566400	0.72604700
C	-4.46108200	0.32869300	0.56609400	O	1.71314300	-2.95093800	0.65469000
H	-3.92910000	-1.94056500	-1.89890800	H	1.58974000	-2.15738000	1.21690200
H	-6.37445700	-2.30215500	-1.53830700	H	0.96099900	-2.41113600	-0.75929500
H	-7.57800200	-0.96928700	0.17568500	H	1.34036000	0.17478800	2.17534400
C1	-6.66978600	1.05353500	1.96120400	O	1.02286200	-0.50578200	1.57811900
H	-3.92746300	1.06477400	1.15299700	H	1.00766900	-0.10467200	0.68934800
C	5.44765800	0.38064700	0.23693500				
C	6.41234300	1.31274100	-0.14818200				
C	5.80927400	-0.96024100	0.37783200				
C	7.72626700	0.91464700	-0.37107200				
H	6.13411700	2.35506700	-0.27575500				
C	7.12178900	-1.35710100	0.14981300				
H	5.05275600	-1.69002800	0.64656400				
C	8.08424400	-0.42144600	-0.22082800				
H	8.46860000	1.64757800	-0.66932100				
H	7.39346200	-2.40240400	0.25491200				
H	9.10746100	-0.73458400	-0.39995200				
H	1.46480900	0.19752400	-0.39341000				
H	0.32754100	-0.17785700	-1.39878300				
O	0.67278500	0.53817000	-0.84653600				
H	-0.80374400	0.74090600	-0.10818100				

TS(2W)

Reactant(2W)

C	-2.60804100	-0.50327800	2.65601500	C	-3.63979800	1.03624200	4.98174700
H	-1.61619600	-0.71512400	2.27209900	H	-2.62379000	1.13351000	5.34377500
H	-3.29103600	0.00451900	1.98185600	H	-4.08358800	1.92801900	4.55765700
C	-2.95570400	-0.85736500	3.89600300	C	-4.39241900	-0.05339900	5.31831600
H	-2.21306000	-1.36708600	4.50813700	H	-3.88191500	-0.87417100	5.81724500
O	0.40238100	-1.92793400	-1.42603900	O	-3.22001800	0.16857000	3.23590300
O	1.37144200	-1.40809700	-2.32486000	O	-2.63761500	-0.13983700	1.61390300
C	1.72546500	-0.13908800	-2.03864100	C	-1.68349800	0.66954800	1.27345700
O	1.42579500	0.45591300	-1.03114100	O	-1.00005000	1.36935000	2.01475800
C	2.56026900	0.42762300	-3.13275400	C	-1.44212000	0.67307600	-0.21463500
C	2.76112100	-0.23352800	-4.34689100	C	-2.29561300	0.01810900	-1.10349500
C	3.54733600	0.35976600	-5.32635800	C	-2.03047900	0.05543100	-2.46719400
C	4.13486400	1.60152500	-5.10813700	C	-0.91967300	0.73704700	-2.95405900
C	3.92411600	2.24829100	-3.89424800	C	-0.07858400	1.38452800	-2.05510700
C	3.14187800	1.67594800	-2.90346500	C	-0.32645400	1.36202800	-0.69116200
H	2.29991300	-1.19717300	-4.52127300	H	-3.15963900	-0.50938700	-0.71889100
H	3.70475700	-0.14545200	-6.27296600	H	-2.69284100	-0.44880200	-3.16283900
H	4.74863500	2.06815800	-5.86961000	H	-0.70606200	0.76993300	-4.01595700
				C1	1.31745500	2.24505900	-2.65859500
				H	0.32258300	1.87271300	0.00901700
				C	-5.80541000	-0.25974500	5.05631800
				C	-6.40601200	-1.44503200	5.50958600
				C	-6.60556500	0.67549300	4.37888000
				C	-7.75772500	-1.68651900	5.30478500
				H	-5.79755000	-2.17898400	6.02949200
				C	-7.95350300	0.43177800	4.17116600
				H	-6.16637000	1.59263500	4.00311100
				C	-8.53627000	-0.74816000	4.63431500
				H	-8.20360900	-2.60771900	5.66483200
				H	-8.55694000	1.16224300	3.64242100
				H	-9.59255300	-0.93368400	4.46958100
				H	-1.05639700	-2.23907100	4.00578300
				O	-1.50042100	-1.55600300	4.51365500
				H	-0.84946000	-0.82891500	4.62572000

H	-2.68069800	-0.57026200	3.62078400
H	0.66026200	1.14605700	4.63730500
O	-0.23767800	0.82173200	4.54367200
H	-0.54545300	1.10790800	3.65134200

Product(2W)

C	-1.12629600	1.01504400	2.87368500
H	-0.07035800	1.15316300	3.08920700
H	-1.81211900	1.77507400	3.23957500
C	-1.63685000	-0.34559000	2.64534800
H	-0.90550400	-1.14993100	2.70053500
O	-1.42038500	0.56433700	1.54244600
O	-0.21695700	0.29941800	-0.80951100
C	1.07962000	0.47350600	-0.97380100
O	1.86914800	0.67935400	-0.06646200
C	1.50812100	0.39782300	-2.39857600
C	0.59345800	0.17113800	-3.42844200
C	1.04033600	0.10795500	-4.74240800
C	2.38994500	0.26875700	-5.03881600
C	3.28981500	0.49456400	-4.00167200
C	2.86451900	0.56114400	-2.68441700
H	-0.45584500	0.04634700	-3.19286900
H	0.33537000	-0.06810800	-5.54763800
H	2.74506600	0.22035200	-6.06149400
Cl	4.98400600	0.69709000	-4.36737400
H	3.56311700	0.73745200	-1.87618800
C	-3.04428900	-0.72382600	2.93297700
C	-3.29145000	-1.84849800	3.72244700
C	-4.12064500	0.02209600	2.44937200
C	-4.59624600	-2.21081400	4.04062900
H	-2.45642300	-2.43865800	4.08813900
C	-5.42414800	-0.34568700	2.76305600
H	-3.92982300	0.87908100	1.81177100
C	-5.66592600	-1.46002200	3.56256300
H	-4.77722500	-3.08533700	4.65715800
H	-6.25518800	0.23623700	2.37745900
H	-6.68419200	-1.74573100	3.80542800
H	1.56941200	-2.87041900	2.85809000
O	1.05542700	-2.16639400	3.25856200
H	1.57170400	-1.35348600	3.10817400
H	-0.49729000	0.38522500	0.14058700
H	3.09546000	0.63817000	2.87315900
O	2.22182600	0.31126300	2.64801700
H	2.10771100	0.48041600	1.69291900