Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Insight on the promiscuous activity of human carbonic anhydrase against the cyanic acid substrate from a combined QM and QM/MM investigation

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Table S2: Cartesian coordinates of the stationary points along the PES of cyanic acid for approach 1 at QM level.

Approach 1		
ES	**TS**	**Carbamate**
C 7.31256800 -1.94609200 -2.54649500	C -6.15306200 -3.45097800 1.88515300	C 6.85358000 -2.59517300 -2.09688400
C 6.15390600 -1.92600400 -1.61577000	C -5.01045900 -3.09825200 1.00196500	C 5.69526700 -2.45657900 -1.17236500
N 6.03751800 -2.76588000 -0.51841900	N -4.08933000 -4.01450400 0.51268400	N 5.34660800 -3.39802000 -0.21506400
C 5.01977600 -1.15981800 -1.59055400	C -4.58287600 -1.89000200 0.52783300	C 4.75620100 -1.46806400 -1.04699000
C 4.87494700 -2.49529800 0.12354200	C -3.15146200 -3.35195900 -0.21009400	C 4.23836100 -2.96336800 0.43775000
N 4.23835700 -1.51716900 -0.50617300	N -3.43275000 -2.05819400 -0.22106600	N 3.86274000 -1.79043000 -0.04316300
C 1.81213300 3.99146100 -2.73489800	C -2.36627300 3.32103700 3.30358000	C 2.25655600 3.89618200 -2.76391000
C 1.61317000 2.56965800 -2.30674800	C -1.98328500 2.05280600 2.61296300	C 1.95719400 2.51672800 -2.27504200
N 0.36185100 2.00013200 -2.18909500	N -0.68098600 1.59516700 2.56620300	N 0.70896300 1.93797300 -2.39536700
C 2.50427200 1.61223200 -1.88584100	C -2.71330500 1.19265000 1.83142100	C 2.73022300 1.60201400 -1.60397100
C 0.51412500 0.76851900 -1.68504900	C -0.65088300 0.53833400 1.74058300	C 0.74972900 0.74270600 -1.78823300
N 1.80742300 0.47641900 -1.48942000	N -1.86542100 0.24678400 1.27282000	N 1.96347400 0.48621600 -1.29471700
C -1.38721900 5.67657300 -0.48368200	C 0.72512800 5.60425100 1.58141700	C -1.08981900 5.70241000 -1.20765800
C -1.18901100 4.17875000 -0.65787700	C 0.67002700 4.08745700 1.48828200	C -1.12820900 4.18011600 -1.28138100
O -0.75220900 3.49708000 0.31761900	O 0.22522300 3.55780800 0.42346500	O -1.03997400 3.53544800 -0.19127000
O -1.44549400 3.71800700 -1.81751300	O 1.04235500 3.46013300 2.52949800	O -1.18340100 3.66627300 -2.44142900
C 4.90647200 0.24618800 2.46307000	C -5.09786000 0.13957500 -2.53716100	C 4.78106100 0.20938300 2.72725300
C 3.67477700 1.09035300 2.33023200	C -4.13706800 1.25295800 -2.24620200	C 3.63785800 1.15318700 2.53342000
N 2.64592600 0.78450500 1.44401700	N -2.99539600 1.07782300 -1.47344200	N 2.58250800 0.87942900 1.67272000
C 3.34423100 2.25274100 2.98139200	C -4.19843700 2.56978000 -2.63021200	C 3.42103300 2.37930500 3.11018400
C 1.72822800 1.74333200 1.55531900	C -2.38764800 2.25780000 -1.38881400	C 1.75338400 1.91732800 1.72594700
N 2.11562100 2.64322600 2.47777900	N -3.08693900 3.18343000 -2.07902500	N 2.22756900 2.84249200 2.58413800
N -3.85419600 -0.57854600 2.34171500	N 3.55363000 0.36837200 -2.63242500	N -3.86048500 -0.20248300 2.59478700
C -4.42550800 0.58987100 1.66510600	C 3.88414500 1.42984800 -1.67929200	C -4.49910300 0.64646900 1.59407900
C -5.00691700 0.22722400 0.28428500	C 4.48906500 0.84563200 -0.38706100	C -4.95308700 -0.01806700 0.26931100
O -5.43229900 1.10056100 -0.47502500	O 4.76269900 1.55876000 0.57794500	O -5.72335000 0.56688900 -0.49421800
C -3.44133100 1.76973100 1.51078500	C 2.72776400 2.38839900 -1.31412100	C -3.63910000 1.88400600 1.25704100
O -2.24644400 1.24012100 0.92970400	O 1.61957900 1.59560900 -0.87235600	O -2.46527900 1.42763100 0.56041500
C -3.14189100 2.45572500 2.84331600	C 2.31997800 3.29789900 -2.47560300	C -3.26317400 2.71382500 2.48614900
N -5.02900600 -1.09824100 -0.01125900	N 4.69744500 -0.50047200 -0.40490000	N -4.45389600 -1.25880600 0.01951700
C -5.52893900 -1.57341400 -1.27789100	C 5.25852300 -1.19994100 0.72300300	C -4.81393400 -2.04182700 -1.13652400
C -6.53327400 -2.70140300 -1.11959700	C 6.33964000 -2.17748600 0.29785600	C -5.54260400 -3.32256400 -0.74821400
O -6.92938300 -3.13678000 -0.05973600	O 6.71106800 -2.34943000 -0.84270700	O -5.83017100 -3.64681300 0.38296100
C -4.41112000 -2.00452500 -2.27291800	C 4.17771300 -1.95081400 1.55344800	C -3.59186800 -2.38962400 -2.03513200
O -3.90258500 -3.30226700 -1.96250000	O 3.57676800 -2.96913500 0.73948300	O -2.64113500 -3.16819500 -1.31048500
C -3.30171100 -0.95770200 -2.38567800	C 3.13085600 -1.01257900 2.15122700	C -2.95685100 -1.15109000 -2.66835900
Zn 2.42989400 -0.69696000 0.03405500	Zn -2.07893900 -0.58240000 -0.58000400	Zn 2.15757800 -0.68937300 0.36797600
O 3.14386400 -3.09636600 2.57358100	O 1.95611300 -5.27093400 0.81057200	O -0.64580400 -4.69456200 0.68730000
H -2.32643800 5.98644400 -0.95012500	H 1.69270000 5.91663200 1.98521100	H -1.54091400 6.14662200 -2.09759200
H -0.58018400 6.20680400 -1.00360900	H -0.03988300 5.94963500 2.28693300	H -0.04272100 6.02754900 -1.15848900
H -3.90414800 2.48683800 0.82190600	H 3.08406900 3.00521500 -0.48050300	H -4.22575900 2.49388800 0.55979000
H -4.05090400 2.89360800 3.27444600	H 3.15757200 3.93066700 -2.79519400	H -4.16443400 3.10700900 2.97141100
H -2.41603500 3.26077500 2.69050500	H 1.50158400 3.95024100 -2.15639400	H -2.63877500 3.55869400 2.17942200
H -2.71826200 1.74649100 3.56408400	H 1.97511900 2.71125100 -3.33550000	H -2.72341000 2.10206300 3.21357600
H -1.69362200 2.00105600 0.64084000	H 1.06302600 2.19324100 -0.31645700	H -1.95824100 2.21069600 0.19753800
H -5.28585500 0.94708600 2.24466300	H 4.68643100 2.03751600 -2.11739000	H -5.42599000 1.03394700 2.03306500
H -2.84829700 -0.61406500 2.18628500	H 2.64460400 -0.03738000 -2.42012700	H -3.02342000 -0.67479100 2.25960100
H -4.88757500 -2.13123200 -3.25306800	H 4.68593800 -2.49699300 2.35757900	H -3.95055200 -3.05394700 -2.83182900
H -2.80126000 -0.81542300 -1.42270200	H 2.61711300 -0.45591000 1.36207400	H -2.64688300 -0.43655800 -1.89843900
H -2.56726600 -1.28991000 -3.12615600	H 2.39679900 -1.59612600 2.71544300	H -2.08487100 -1.44984900 -3.25829800
H -3.70412400 0.01353400 -2.69072700	H 3.59567300 -0.28165400 2.81980700	H -3.66582900 -0.63748400 -3.32656300
H -3.54728600 -3.32055000 -1.05882500	H 3.11113900 -2.54873100 -0.00903900	H -2.26817300 -2.64053300 -0.57516900
H -6.06006000 -0.72671700 -1.73934200	H 5.72388200 -0.45340300 1.38469300	H -5.51769200 -1.43739600 -1.72743400
H -4.76069900 -1.73355900 0.73490900	H 4.61131700 -0.95444600 -1.31035000	H -3.85061600 -1.68153700 0.71299700
H 7.16974200 -1.19888600 -3.33052300	H -6.71619300 -2.54885700 2.13534400	H 6.90220700 -1.72437300 -2.75439700
H 7.42853900 -2.92099500 -3.03499000	H -5.81464000 -3.90232000 2.82561300	H 6.76598300 -3.48576000 -2.73035300
H 6.70248100 -3.47361500 -0.23915000	H -4.08823700 -5.00932600 0.68832500	H 5.81817400 -4.27546700 -0.04491500
H 4.71094500 -0.39532100 -2.28699200	H -5.01463300 -0.91664900 0.70249300	H 4.64952500 -0.56622900 -1.62947300
H 4.53240200 -2.99604400 1.02293200	H -2.25917100 -3.79180600 -0.64155900	H 3.74239700 -3.51651200 1.22209200
H 1.40665300 4.68436100 -1.99076300	H -3.45331800 3.44241500 3.29569300	H 3.30792500 4.13856400 -2.58522800
H 1.30772800 4.19971700 -3.68369700	H -1.92200800 4.18713200 2.80184100	H 1.63884300 4.64008300 -2.25193800
H -0.55275700 2.61682900 -2.12338500	H 0.17055800 2.25430100 2.70008000	H -0.18770900 2.51603600 -2.56009800
H 3.58014300 1.67827200 -1.81254800	H -3.77121700 1.21202200 1.61401300	H 3.76307300 1.69120600 -1.29887100
H -0.31421900 0.12008200 -1.43705100	H 0.25749400 0.02956300 1.45502800	H -0.10907300 0.09791200 -1.68279500
H 4.64617300 -0.78327900 2.73186700	H -4.58177600 -0.72583600 -2.96487200	H 4.43424700 -0.76127000 3.09862900
H 5.47283600 0.22359500 1.52600300	H -5.61130800 -0.19742700 -1.63108700	H 5.31912000 0.03428300 1.78976200
H 3.86467100 2.81771800 3.73858900	H -4.91582400 3.10648600 -3.23098700	H 3.99331900 2.94194100 3.83082600
H 0.80967400 1.84961800 0.99239400	H -1.48185700 2.48753200 -0.83754200	H 0.83276100 2.03123000 1.17207700
H 1.58099400 3.46603500 2.72088000	H -2.82455700 4.15469500 -2.16759600	H 1.76768200 3.71615000 2.79791000
H 2.75268300 -3.54392700 3.33255400	H 2.57254900 -4.52170600 0.94949000	H -1.10702100 -4.92579600 -0.13071800
H 2.39617000 -2.82834400 1.97954600	H 2.49927700 -5.99492700 0.47727200	H -1.15063900 -3.92861900 1.02417100
O 1.40856100 -2.20379000 0.68854700	O -0.50757300 -1.12117000 -1.48436400	O -0.47438800 -0.04450900 1.18504200
H 1.36072500 -2.89516400 0.01448600	H 0.12668500 -0.39404800 -1.57898600	H -1.36796300 0.41010600 1.05674800
C -1.91803800 -3.13854600 1.26530300	C 0.75875800 -2.74945700 -1.08337000	C -0.50525000 -1.37960400 1.01822100
N -1.00568200 -2.56955100 1.81210000	N -0.05024000 -3.59321300 -0.66443300	N 0.70439200 -1.89864400 0.78999400
H -0.05683800 -2.33504400 1.41835500	H 0.46040100 -4.39754900 -0.27060800	H 0.66307700 -2.90568000 0.65311900
O -2.86920000 -3.68670600 0.81244600	O 1.79403900 -2.24618600 -1.40275600	O -1.59521600 -2.01463100 1.07598400
H 5.55736900 0.65107100 3.24273300	H -6.84583000 -4.15418000 1.40701900	H 5.48954200 0.61377200 3.45511200
H 8.25370000 -1.71447500 -2.03348400	H -2.02745700 3.33677000 4.34489700	H 7.80532500 -2.65972300 -1.55627100
H 2.87827100 4.20296600 -2.85581000	H 0.55474900 6.07619900 0.61076100	H 2.05866500 3.99592400 -3.83658600
H -1.37636200 5.96355600 0.57029800	H -5.85668000 0.47139100 -3.25077200	H -1.58897900 6.06497600 -0.30491300
H -6.90312400 -3.11822100 -2.08048200	H 3.53263000 0.71475400 -3.58532700	H -4.49917300 -0.90625400 2.95080300
H -4.01843700 -0.55338300 3.34170100	H 6.78534500 -2.75813800 1.13483200	H -5.80841900 -3.97420500 -1.61002500

Table S2: Cartesian coordinates of the stationary points along the PES of cyanic acid for approach 2 at QM level.

Approach 2		
ES	**TS**	**Carbamate**
C 6.77352100 -1.33387100 -2.63064900	C 6.64912 -0.89532 -3.21744	C 6.55830600 -2.31346500 -2.64396900
C 5.62326500 -1.43964700 -1.68841800	C 5.56603 -1.07962 -2.20674	C 5.43252000 -2.20959000 -1.67031900
N 5.63214400 -2.21753600 -0.53842000	N 5.44401 -2.21254 -1.41081	N 4.86730900 -3.30028200 -1.02415100
C 4.38844700 -0.84740300 -1.69708700	C 4.52275 -0.27728 -1.82893	C 4.72469200 -1.13091900 -1.20885800
C 4.44268100 -2.07505200 0.09835700	C 4.36581 -2.06394 -0.59956	C 3.86587400 -2.86018100 -0.22146800
N 3.67004600 -1.24351500 -0.58253200	N 3.79150 -0.89504 -0.82917	N 3.76117400 -1.54465300 -0.30695300
C 1.04473500 4.38111500 -2.58622900	C 1.28303 4.93712 -1.89347	C 2.07605300 3.92789300 -2.91252900
C 0.95512800 2.92668100 -2.25987900	C 1.15396 3.48974 -1.54150	C 1.72524600 2.70284600 -2.13278500
N -0.24942400 2.25726400 -2.19996600	N -0.04856 2.82166 -1.62771	N 0.43777700 2.21577100 -2.07054500
C 1.91642500 2.00858600 -1.91151700	C 2.06542 2.57257 -1.07497	C 2.48817700 1.85719600 -1.36448500
C -0.00151200 1.00135500 -1.80633500	C 0.14906 1.56326 -1.21017	C 0.44370100 1.13221700 -1.28279100
N 1.30865400 0.79501100 -1.62271900	N 1.42665 1.35863 -0.86779	N 1.67486900 0.86662800 -0.83285000
C -2.81880400 5.59622100 -0.55122400	C -3.22638 5.90866 -0.52525	C -2.05863100 5.95963200 -1.73582600
C -2.30967900 4.16840300 -0.71180400	C -2.66090 4.50830 -0.74430	C -1.79781700 4.45975900 -1.63973000
O -1.88518600 3.55009800 0.31179600	O -2.74990 3.66762 0.18709	O -1.97699900 3.89619100 -0.52665300
O -2.31637900 3.71077500 -1.89853300	O -2.08446 4.30739 -1.86891	O -1.35850400 3.89032200 -2.69489500
C 4.45646300 0.83160400 2.21765700	C 5.06986 0.82166 1.91366	C 5.29564300 0.65352200 1.97995100
C 3.11745400 1.49983500 2.12269900	C 3.75186 0.89811 2.61236	C 4.02454500 1.12135600 2.60622600
N 2.08150800 1.03949000 1.31344300	N 2.55764 0.49877 2.02379	N 2.77795900 0.70642300 2.15612200
C 2.68882300 2.63387600 2.76711500	C 3.48216 1.33869 3.88182	C 3.84331800 1.99414300 3.64820000
C 1.06579100 1.88422100 1.46823800	C 1.59106 0.69682 2.91695	C 1.86397200 1.32066400 2.90448800
N 1.39302300 2.85658000 2.33958000	N 2.11650 1.20245 4.05210	N 2.47486100 2.10420600 3.81872400
N -4.07933200 -1.27462400 2.21504800	N -4.04218 -1.28749 2.19496	N -4.00434800 -0.09400300 2.56227100
C -4.57918600 -0.43694500 1.12685200	C -4.74233 -0.46491 1.20432	C -4.60565800 0.44988000 1.35665700
C -4.36572000 -1.10003200 -0.25291700	C -4.73563 -1.13198 -0.18390	C -4.76344300 -0.48348800 0.13320900
O -4.79682800 -0.57515700 -1.28044400	O -5.34105 -0.65081 -1.13876	O -5.47450400 -0.14957300 -0.81552600
C -4.10109400 1.03682400 1.09753800	C -4.27694 1.00574 1.05621	C -3.94765000 1.77474600 0.90704000
O -2.66786300 1.05671300 0.99322500	O -2.95447 1.03184 0.49207	O -2.62201000 1.50567700 0.40971000
C -4.56646700 1.83179100 2.32165900	C -4.30538 1.76721 2.37985	C -3.89932500 2.82672400 2.01454400
N -3.71422300 -2.29683200 -0.23404900	N -3.98692 -2.27421 -0.26374	N -4.12320800 -1.69223700 0.17208300
C -3.70175000 -3.19242700 -1.37055500	C -3.86747 -3.03551 -1.48586	C -4.41757900 -2.71242500 -0.81004500
C -3.84870800 -4.62732000 -0.89563700	C -3.83271 -4.52405 -1.18346	C -4.80054700 -4.02840200 -0.15300500
O -3.97019400 -4.96463400 0.26265800	O -3.97101 -5.00723 -0.08144	O -4.87396500 -4.20490600 1.04489200
C -2.43813700 -3.09462600 -2.28249800	C -2.59941 -2.61595 -2.29428	C -3.31483800 -2.94906600 -1.87550500
O -1.25003900 -3.33239000 -1.54349400	O -1.48140 -2.55576 -1.39977	O -2.18391900 -3.65685400 -1.34469900
C -2.39227400 -1.80393200 -3.09938700	C -2.77808 -1.30129 -3.04931	C -2.88557300 -1.65507000 -2.56083900
Zn 1.82996800 -0.47820400 -0.12535000	Zn 2.11385 -0.23932 0.14691	Zn 2.17757400 -0.49113200 0.54737300
O -1.02318700 -0.72858900 2.28655300	O -1.09740 -0.32521 1.96338	O -0.94785600 0.47078900 2.21243600
H -3.72499500 5.73901500 -1.14622000	H -2.40097 6.58446 -0.27006	H -2.38872100 6.23115300 -2.74167300
H -2.06393200 6.28889900 -0.94233400	H -3.94959 5.91888 0.29273	H -1.11879300 6.48975700 -1.53756200
H -4.52044100 1.48185800 0.18702100	H -4.96017 1.47915 0.34121	H -4.54991700 2.14501900 0.06968100
H -5.66150500 1.86661800 2.37286700	H -5.31957 1.78371 2.79937	H -4.91202100 3.06927400 2.35881400
H -4.19391700 2.85874100 2.26062800	H -3.98265 2.79744 2.21171	H -3.43440400 3.73649700 1.62502200
H -4.18581000 1.38549800 3.24723800	H -3.63459 1.30593 3.11273	H -3.32897700 2.46345100 2.87349800
H -2.38337900 1.96097500 0.69515800	H -2.76294 1.98782 0.27715	H -2.30266000 2.34798700 -0.02695500
H -5.67204900 -0.39578400 1.22110600	H -5.79983 -0.42087 1.49146	H -5.64392100 0.71561900 1.59679600
H -3.08711200 -1.14491900 2.40459600	H -3.04952 -1.06112 2.27144	H -2.99395800 -0.19884800 2.54376200
H -2.50056200 -3.93805400 -2.98454700	H -2.36096 -3.41571 -3.00766	H -3.74807500 -3.62405400 -2.62639000
H -2.43291200 -0.92189600 -2.45525000	H -3.01043 -0.47919 -2.36797	H -2.48303800 -0.94315600 -1.83508400
H -1.47327000 -1.78120500 -3.69347800	H -1.85546 -1.06573 -3.58954	H -2.11816600 -1.87353900 -3.31011300
H -3.25259500 -1.73912500 -3.77288300	H -3.59755 -1.37392 -3.77263	H -3.73531500 -1.17565400 -3.05660400
H -0.99412900 -2.55687200 -1.00729400	H -1.81685 -2.15860 -0.57761	H -2.04425900 -3.51235000 -0.37796500
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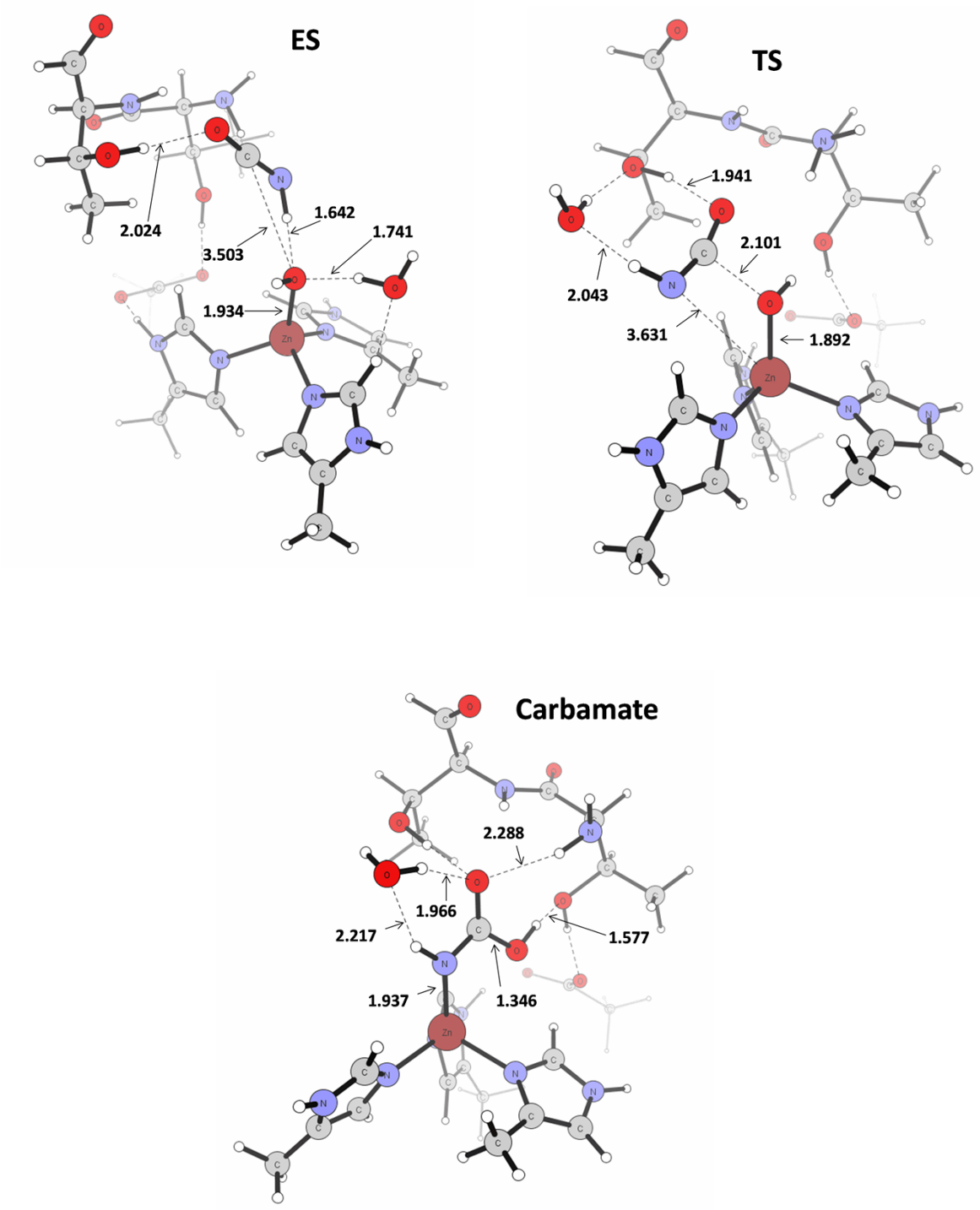

Figure S1. QM optimized structures of the stationary points along the PES of cyanic acid for approach **1**. All bond lengths are given in Å

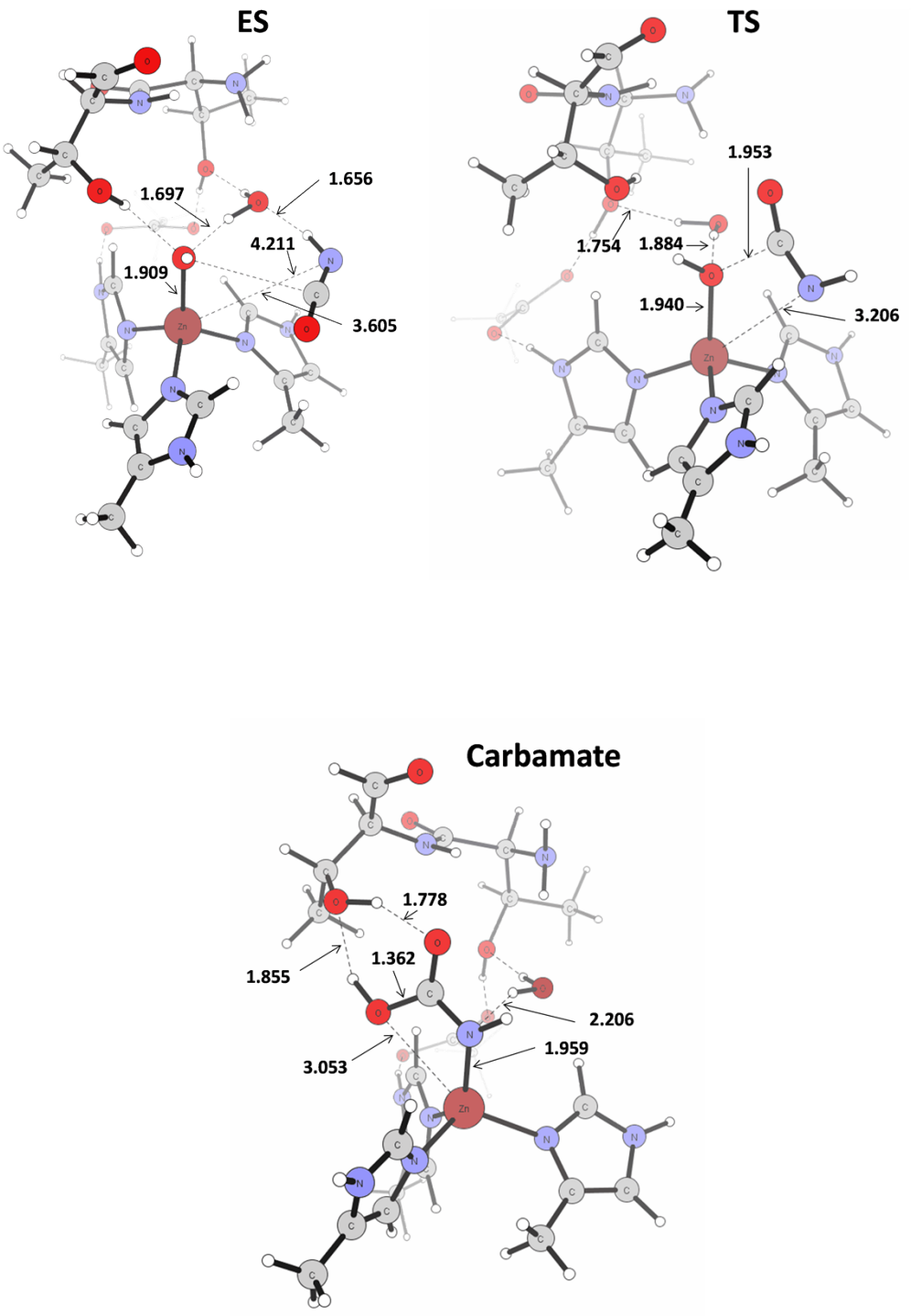

Figure S2. QM optimized structures of the stationary points along the PES of cyanic acid for approach **2**. All bond lengths are given in Å

MD Procedure

MD simulations were carried out with NAMD[1] using CHARMM[2] force field. The available crystal structure of HCO_3^--hCAII complex (PDB Code 2VVB) was used as starting structure, while since the lack of crystal structure of the analogue carbamate-hCAII, the minimized energy structure of carbamate was docked into the hCAII (PDB code 2CBA) using Autodock[3]. All ligands required custom parameters for the force field. They were obtained from parameters by similar models through analogies (carbon dioxide) and parameterized in order to create the topology and input files required by the CHARMM calculations starting from the Gaussian output files (carbamate). The charges for the ligands atoms, for the metal core and for the coordinated histidine residues were set using the NBO charges arising from DFT calculations.
With the aim to reproduce the natural flexibility of the enzymatic metal core and to preserve the zinc coordination a combination of bonded and non-bonded description was used: harmonic constraints were introduced using the Colvars module of NAMD with QM/MM values regarding bonds, angles and dihedral.[see Table S1] [4]

A water layer of 16 Å was built around each studied enzyme-product complex creating a water box of 81 x 77 x 87 $Å^3$ for hCAII-carbamate and 80 x 78 x 89 $Å^3$ for hCAII-HCO_3^-. The resulting number of atoms was 51053 for hCAII-carbamate complex and 52101 for the hCAII-HCO_3^- one. Due to the neutral charge of the studied systems no further neutralization was needed. SHAKE [5] algorithm was practiced in order to constrain all bonds involving hydrogen atoms. Periodic boundary conditions were used. The long-range electrostatic interactions were evaluated by Particle Mesh Ewald (PME) method [6]. The supramolecular systems obtained including protein, waters and the ligand (HCO_3^- and carbamate) were minimized using the conjugate gradient algorithm: in first instance, minimizing the water molecules keeping the protein and ligand fixed, and then minimizing the entire system.

A time step of $\Delta t = 2$ fs was used for both systems. A cutoff of 12 Å for non-bonded interactions was applied and a switching scheme was used. Scaled 1–4 parameters were enabled for 1–4 interactions. A first equilibration of 60 ps was performed on the minimized models by increasing temperature until to 300 K in increments of 20 K. Then a simulation time equal to 10 ns was performed in the NPT ensemble with a Langevin dampening coefficient of 5 ps^{-1} controlling pressure with the Langevin piston pressure control.

Table S3 : Parameters for the zinc coordination in the bicarbonate–hCAII complex.

Atoms			Force Constant	Equilibrium
Bonds			k	r_e
Zn		N_{119}	30 kcal/mol/ Å^2	2.07 Å
Zn		N_{94}	30 kcal/mol/ Å^2	2.01 Å
Zn		N_{96}	30 kcal/mol/ Å^2	2.01 Å
Angles			k	θ_e
N_{119}	Zn	N_{96}	23 kcal/mol/ rad^2	96.9°
N_{96}	Zn	N_{94}	23 kcal/mol/ rad^2	107.2°
N_{94}	Zn	N_{119}	23 kcal/mol/ rad^2	118.2°
$O_{bicarbonate}$	Zn	N_{119}	0.05 kcal/mol/ rad^2	104°
$O_{bicarbonate}$	Zn	N_{94}	0.05 kcal/mol/ rad^2	108°
$O_{bicarbonate}$	Zn	N_{96}	0.05 kcal/mol/ rad^2	120°
Improper Dihedrals			k	ϕ_0
Zn	N_{119}	N_{96} N_{94}	25 kcal/mol/ rad^2	0

Table S4 : Parameters for the zinc coordination in the carbamate –hCAII complex.

Atoms			Force Constant	Equilibrium
Bonds			k	r_e
Zn		N_{119}	30 kcal/mol/ Å^2	2.13 Å
Zn		N_{94}	30 kcal/mol/ Å^2	2.01 Å
Zn		N_{96}	30 kcal/mol/ Å^2	2.01 Å
Angles			k	θ_e
N_{119}	Zn	N_{96}	23 kcal/mol/ rad^2	94.5°
N_{96}	Zn	N_{94}	23 kcal/mol/ rad^2	103.4°
N_{94}	Zn	N_{119}	23 kcal/mol/ rad^2	110.1°
$O_{carbamate}$	Zn	N_{119}	0.05 kcal/mol/ rad^2	109.7°
$O_{carbamate}$	Zn	N_{94}	0.05 kcal/mol/ rad^2	123.7°
$O_{carbamate}$	Zn	N_{96}	0.05 kcal/mol/ rad^2	113.6°
Improper Dihedrals			k	ϕ_0
Zn	N_{119}	N_{96} N_{94}	25 kcal/mol/ rad^2	0

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