

Supporting Information for

Antibiotic binding to monozinc CphA β -lactamase from *A. hydrophila*: QM/MM

and DFT studies

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Cartesian coordinates of DFT models

I. Biapenem (B3LYP/6-31+G(d))

S	0.000000000000	0.000000000000	0.000000000000
O	0.000000000000	0.000000000000	3.023854000000
O	1.972920326172	0.000000000000	4.135948847963
O	3.744107984494	-2.733317837124	3.457579685387
O	6.680681282693	-1.307784732058	1.676282911332
N	3.345748207287	-0.914710646092	1.939814816685
N	-0.111255469115	3.309254506899	-0.487916553892
N	-1.772225063544	4.601109534623	0.162177979337
N	-1.246003169137	2.864687635991	-1.085039601675
C	2.703075475245	-1.028390814254	-0.390896515094
C	1.621412291294	-0.437008501879	0.536675256395
C	2.016949495022	-0.484026423354	1.841534196713
C	3.924810292954	-1.095271037574	0.580075728033
C	4.588825820638	-2.419287596632	1.069974188939
C	3.871014971977	-2.159509209942	2.411060535478
C	6.126207421572	-2.491048298372	1.093702388580
C	6.715078598898	-2.625128360735	-0.306924883872
C	2.252283072118	-2.353904793284	-1.030940217535
C	1.207079048404	-0.143279377945	3.042376753487
C	0.372089798380	1.192043323540	-1.371576125325
C	1.054561916392	2.484902408445	-0.857721293274
C	-0.461443113459	4.360265576133	0.264853435337
C	-2.236927976754	3.666474867266	-0.672305061349

C	-0.987649474202	1.682049081930	-1.929546834777
H	2.949703705472	-0.330301252213	-1.201746703225
H	4.654640877105	-0.311460332053	0.362357974938
H	4.184089537057	-3.324097387780	0.603637094361
H	6.405637458422	-3.369564765027	1.691806612443
H	7.805018041304	-2.695300043876	-0.246467062249
H	6.468645296346	-1.749317475003	-0.919090314006
H	6.335139992072	-3.522824364041	-0.807731502030
H	1.972719230418	-3.094000146884	-0.273770934907
H	1.380734667700	-2.201335441576	-1.675964870958
H	3.056444476168	-2.772111898409	-1.646430240073
H	6.675719792667	-1.381811243827	2.643725188298
H	0.966134658339	0.723142940728	-2.158398305645
H	1.687016857333	2.320897283057	0.016554085220
H	1.620296562949	3.004108421853	-1.639425581638
H	0.241509127526	4.918996077383	0.868141618798
H	-3.266360313320	3.546996354444	-0.982844080745
H	-1.798643699114	0.959914672867	-1.813473518769
H	-0.921517452865	1.998603544775	-2.975288464156
H	1.385266297914	0.168252847008	4.897842669023

II. Active-site Model for Apo Enzyme (B3LYP/6-31+g(d))

C	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.096986000000
H	1.047079315988	0.000000000000	-0.324004638855
C	-0.707019273102	-1.257974772126	-0.504753623841
O	-1.778995128196	-1.157235088085	-1.130921878129
O	-0.101272446965	-2.360352831541	-0.217851761955
H	-0.504966754512	0.899116142451	-0.361813395616
C	-0.854567216516	-3.046361218747	-3.910813902014
H	0.162134102780	-2.639888747323	-3.874038067061
H	-1.128961948178	-3.197130398946	-4.961028678923
S	-0.956981196351	-4.679427325705	-3.050491892553
H	-1.536791978025	-2.320645822162	-3.462208861088
C	-4.330978946170	-7.186047384954	-3.129439373911
H	-3.861639322666	-8.167897976000	-3.259932629700
H	-5.130897693137	-7.078931286913	-3.878362444701
N	-4.808320102696	-7.051452370816	-1.742146825709
H	-5.272859263284	-6.143145296282	-1.606169459352
H	-3.519043857868	-6.898357801318	-0.684563089056
H	-5.496574008632	-7.768449151672	-1.518561933808
C	2.011040704410	-8.960040588005	-0.190140924775
H	1.290812395770	-9.788984621833	-0.180124882005

H	2.471604791748	-8.930938834895	-1.182543750011
N	0.621842602249	-7.412194487631	1.255855902647
H	0.206620871710	-8.114455056456	1.864546935836
C	1.349498774041	-7.651776697046	0.097210104894
H	2.798400881962	-9.194496511967	0.539420746399
C	0.124064199121	-6.154154813776	1.180736790813
H	-0.540056471162	-5.733304577892	1.919875905202
N	0.503167984603	-5.557376987419	0.065846619529
C	1.273779118891	-6.482030415468	-0.617316484791
H	1.681455782065	-6.251916695447	-1.591473832949
Zn	-0.796397666365	-4.106857400307	-0.839822405151
C	-3.092739032167	-5.453305614277	0.543127192259
O	-2.319851586698	-4.441387868275	0.535238747403
O	-2.690813017350	-6.529956002706	-0.195811584901
O	-4.173252715955	-5.526231713468	1.184415705807
O	-6.013005302530	-4.439159572900	-0.735954767761
H	-5.521169478356	-3.590626703889	-0.812231501382
H	-5.650479630532	-4.799242636427	0.097817595357
O	-4.209600282624	-2.296780151010	-0.163801566857
H	-3.683936483462	-2.941352830497	0.349871891712
H	-3.511250690944	-1.824298509456	-0.664485629511
O	-4.467331267651	-7.719156961078	2.781495012331
H	-4.553318963395	-7.305828657007	3.652840470798
H	-4.445316963920	-6.952876127428	2.145991243268
O	-1.917551546762	-8.581882407435	1.850945689325
H	-2.759727346254	-8.470933710740	2.345308862181
H	-2.070316259097	-8.029430484109	1.057073089988
H	-3.569115490535	-6.422299906993	-3.314872680901

III. Active site Model for Enzyme-Biapenem Complex (B3LYP/6-31+G(d))

C	0.000000000000	0.000000000000	0.000000000000
H	0.000000000000	0.000000000000	1.096603000000
H	1.047050348684	0.000000000000	-0.325448425544
N	-0.318881565855	-2.483134537032	-0.246335700649
C	-0.728512706325	-1.192938267926	-0.535486741359
C	-1.164059551825	-3.287308881333	-0.858891101318
H	-1.133205213957	-4.368331678316	-0.842383916273
H	-0.465217508094	0.930352791710	-0.342439401243
N	-2.110887875960	-2.581721424080	-1.537863407575
H	-2.866773110402	-2.967882139001	-2.085926391620

C	-1.843911345386	-1.238083246047	-1.339251558139
H	-2.454417283113	-0.460900483796	-1.775044751129
C	4.292404501282	-3.154841451375	-1.465315570768
H	5.210498165616	-2.663102028568	-1.794232401581
H	3.574228818077	-3.165271676046	-2.294697849375
C	4.583575805252	-4.586543985743	-1.037580762274
O	3.589638368933	-5.197611659279	-0.447705111696
O	5.682518347637	-5.108080128702	-1.263689751811
H	3.829914186880	-2.591574604382	-0.648261187911
C	0.559588563879	-6.975679094255	0.491483767086
H	0.428502579243	-6.655213686230	-0.546579747130
H	-0.377247738720	-7.420580206795	0.841711356939
S	1.888126773858	-8.257109463926	0.587159288180
H	0.794818878687	-6.101487401251	1.103659575037
C	5.481980100484	-11.286134800472	-3.454022061750
H	6.370321599463	-11.861439187484	-3.161895884264
H	4.604056127514	-11.903711478228	-3.243708791544
N	6.347774429978	-9.000674458613	-2.777005083519
H	7.196792154324	-9.033671310882	-3.325138126324
C	5.381526140303	-9.997062794352	-2.706104862143
H	5.525585261539	-11.129374506048	-4.539896001040
C	5.968765987530	-7.963665889937	-1.989101399907
H	6.510090661888	-7.036905815881	-1.862217194540
N	4.810535830091	-8.238662702808	-1.414375516964
C	4.434273873952	-9.497070271780	-1.850233857609
H	3.508098136124	-9.945082061794	-1.518940560632
S	8.373903739698	-5.404929286751	3.413986284793
O	5.665855242777	-7.909263809199	3.706199810701
O	5.061278287504	-7.510430241494	1.592012080885
O	2.758293782520	-5.638616430954	4.421346959187
N	4.439635240901	-4.862394181535	2.922062784368
C	6.263217762547	-3.418341430936	3.480108663166
C	6.684668460522	-4.879375042495	3.270272666980
C	5.623753196378	-5.656770113291	2.969235043328
C	4.783553734422	-3.413273057803	3.030743451719
C	3.592393399189	-3.258395028721	4.022736188626
C	3.433312098962	-4.773994576153	3.881235107481
C	5.477714845658	-7.141179790169	2.735864443540
C	8.341161007774	-6.338867421567	5.000857299673
H	6.870690059154	-2.730996437009	2.882310891106
H	4.628967960719	-2.897542562388	2.081038996916
H	3.858493920284	-2.956979687588	5.041013715576
H	7.612880732506	-7.149413242071	4.939575608941
Zn	3.845924628743	-7.098201255030	0.024358170979

O	1.988730738943	-3.547123466761	1.294392623126
H	2.468672610584	-4.128081963587	0.667475367559
H	1.233317651108	-3.174235900601	0.792289206532
C	2.101151845441	-9.348231367287	4.496562445027
H	2.456587264746	-9.304693632892	5.527940453065
H	1.042058024225	-9.086608498953	4.458582440713
N	2.867718772615	-8.385921492080	3.668663758507
H	2.538270808788	-8.386558326540	2.661189553202
H	3.890923805436	-8.572490534137	3.675981104764
H	2.767209021018	-7.404425830310	4.005328578364
H	2.242284310545	-10.354553439602	4.097673337988
H	2.744415194251	-2.681462842128	3.648540900544
H	6.401052182367	-3.132379946448	4.533911128615
H	8.111709409733	-5.675750569995	5.839787165944
H	9.348417075105	-6.746872312966	5.131536212065