

Supplementary Material

Exploring clomiphene inclusion in β -cyclodextrin: a computational approach

Hélio F. Dos Santos^{A,*}, *Eloah P. Ávila*^A and *Cleber P. A. Anconi*^B

^ADepartment of Chemistry, Federal University of Juiz de Fora, Juiz de Fora, MG, 36036-900, Brazil

^BDepartment of Chemistry, Institute of Natural Sciences, Federal University of Lavras, Lavras, MG, 37200-900, Brazil

*Correspondence to: Email: helio.santos@ufjf.br

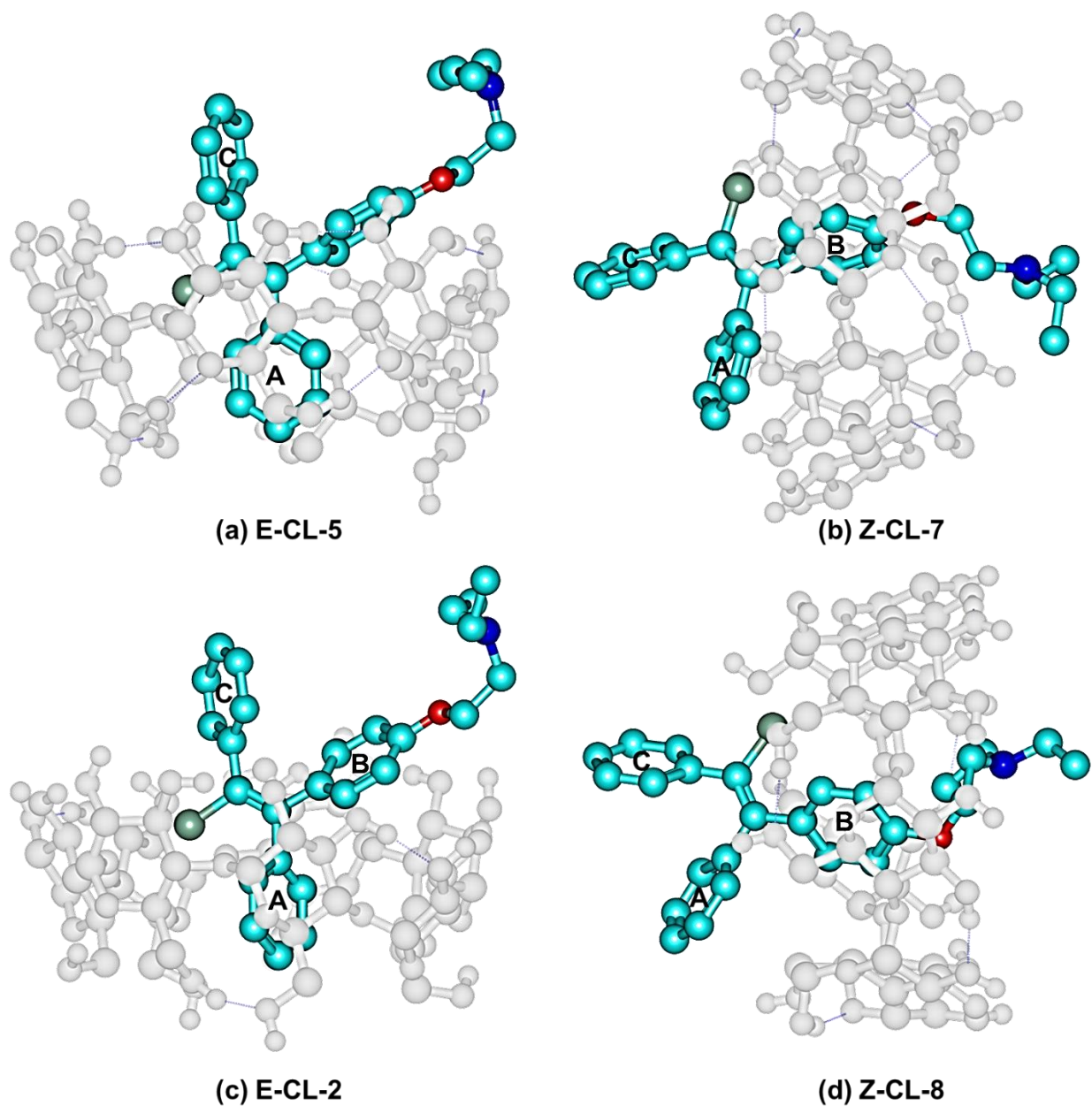


Figure S1. Most stable inclusion complexes in gas phase at GFN2-xTB level (**a,b**). The ΔG_i^{gas} was (kcal mol⁻¹) -3.49 (*E*-CL-5) and -4.79 (*Z*-CL-7). Most stable inclusion complexes in aqueous solution at GFN2-xTB-ALPB level (**c,d**). The $\Delta G_i^{sol-OPT}$ was 2.52 kcal mol⁻¹ (*E*-CL-2) and 2.04 kcal mol⁻¹ (*Z*-CL-8).

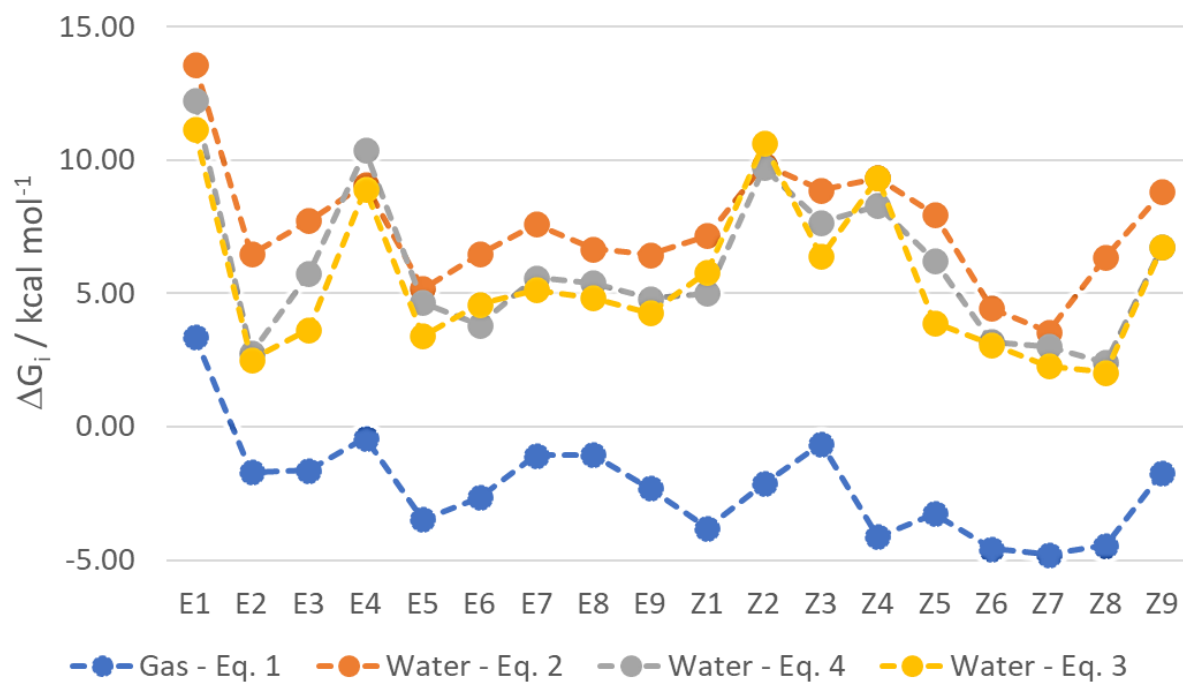


Figure S2. Inclusion free energy calculated from various approaches at the GFN2-xTB level. Eqn 1–4 are discussed in the main text. This figure illustrates the role of the solvent, as well as the different methods used to account for solvation energy within the continuum model.

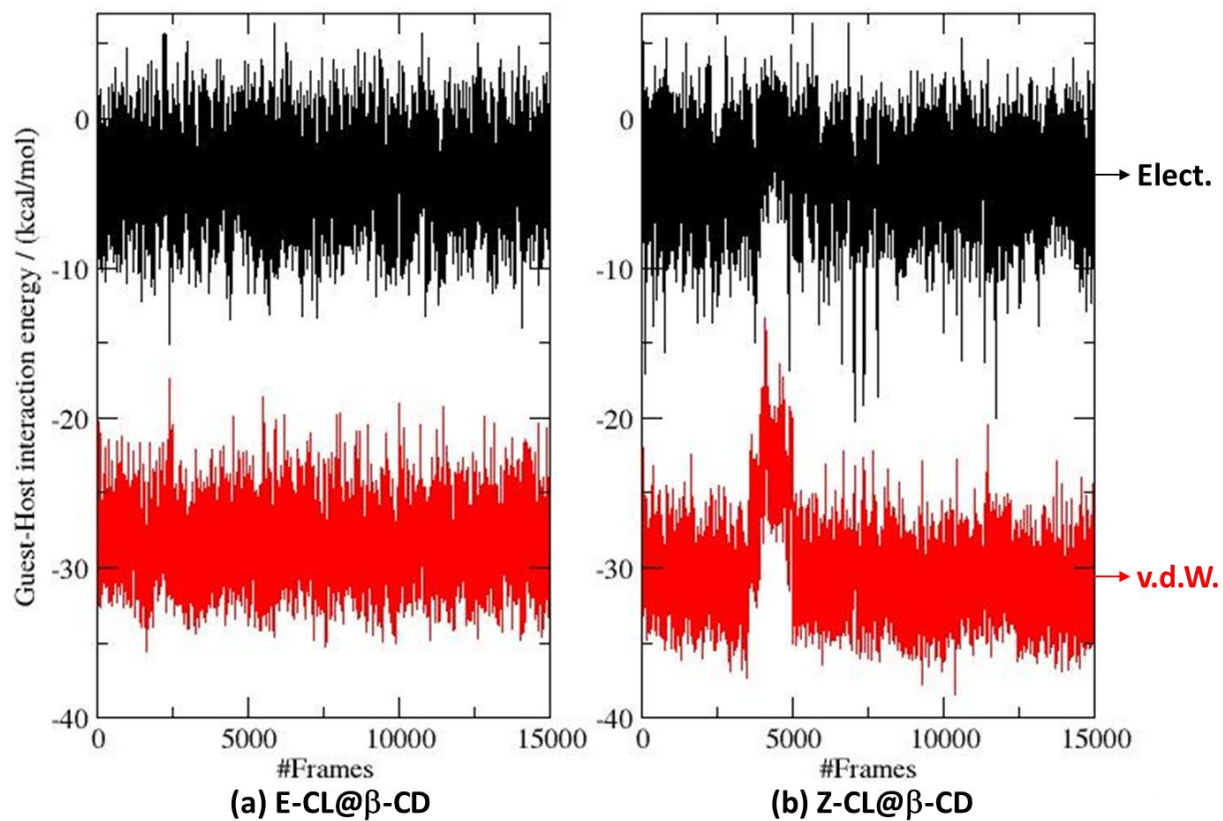


Figure S3. Pair interaction energy calculated for the CL@ β -CD system within a cutoff of 12 Å. The electrostatic contributions are shown in black, whereas the van der Waals contributions are depicted in red, with both calculated in the gas phase using classical potentials.

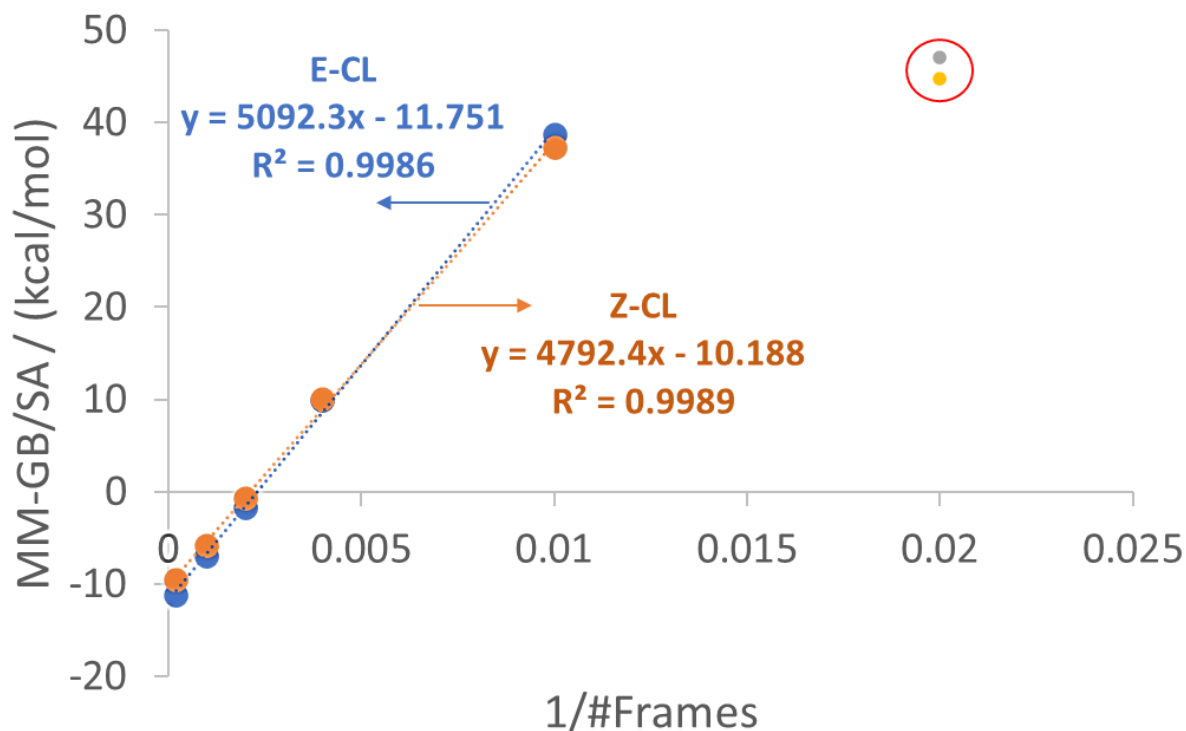


Figure S4. Correlation between the MM-GB/SA binding free energy and the reciprocal of the number of frames selected from the MD trajectory. The points indicated by the red circle correspond to number of frames = 50 and were excluded from the linear fitting. The extrapolated binding free energies for number of frames $\rightarrow \infty$ are $-11.75 \text{ kcal mol}^{-1}$ for *E*-CL@ β -CD and $-10.19 \text{ kcal mol}^{-1}$ for *Z*-CL@ β -CD.

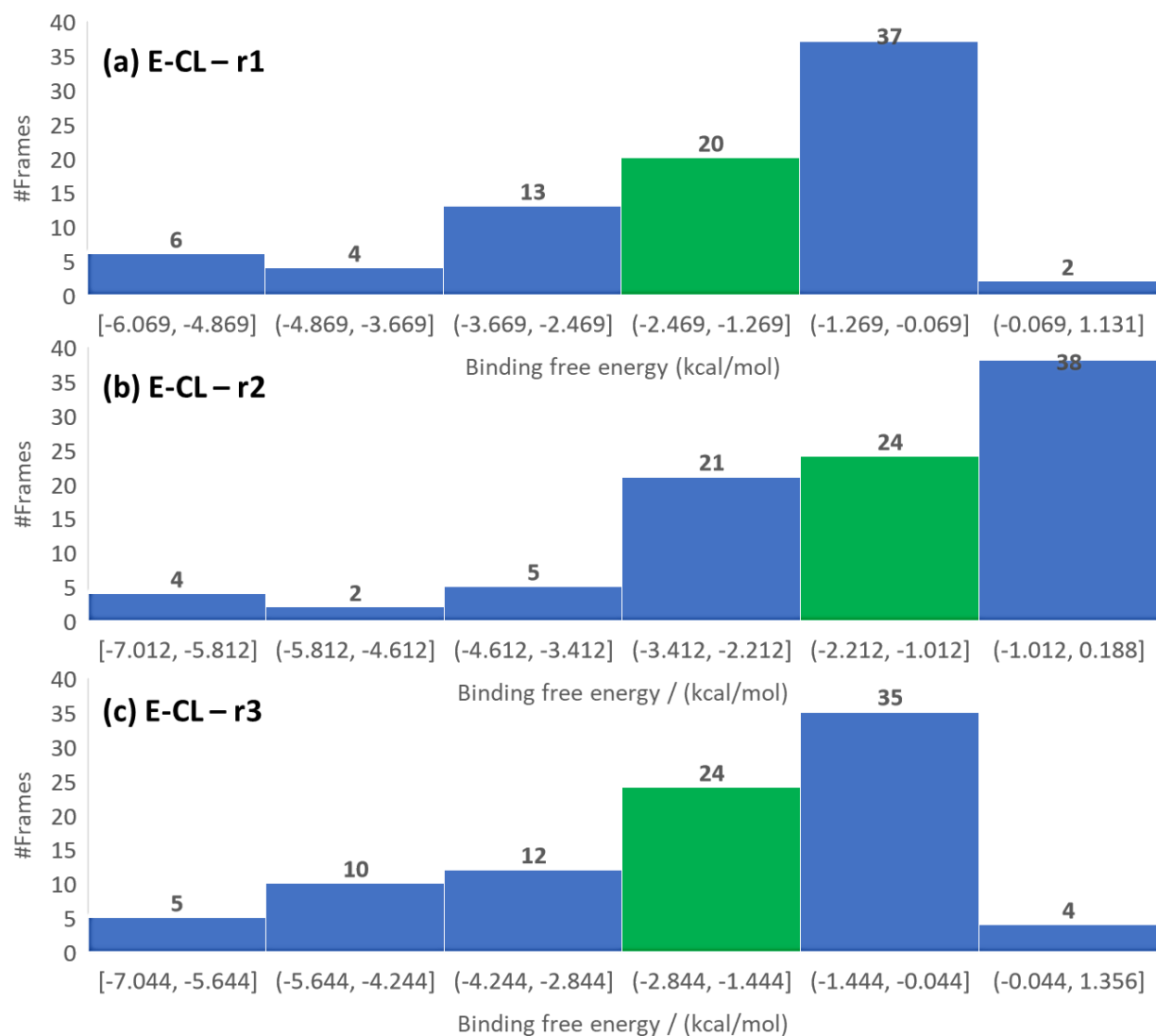


Figure S5. Binding free energy distribution for *E*-CL@ β -CD complexes (**a–c**) and *Z*-CL@ β -CD complexes (**d–f**). The labels r1, r2, and r3 correspond to the three independent MD trajectories. The average values are within the green bar.

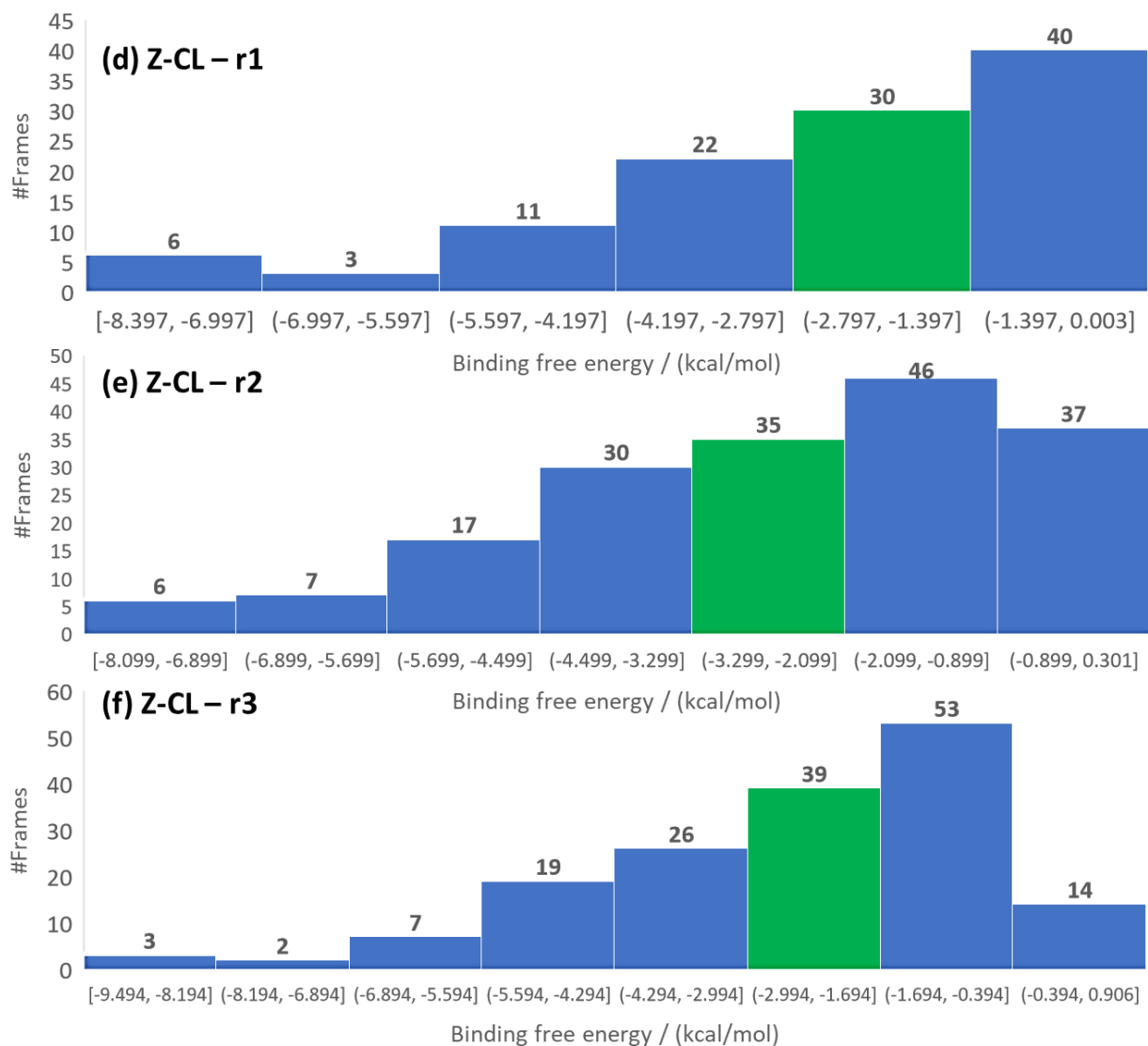
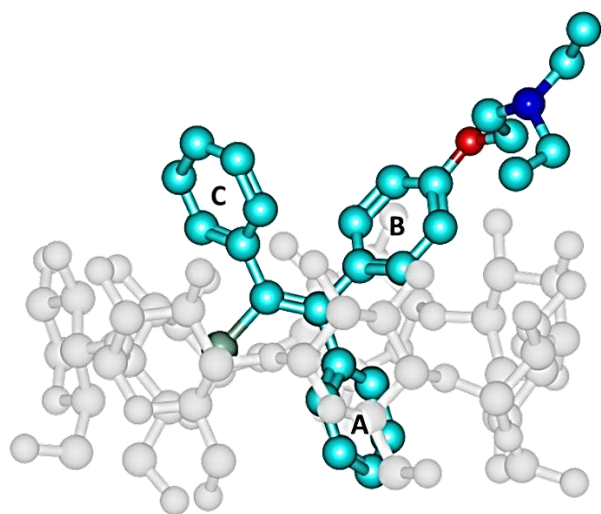
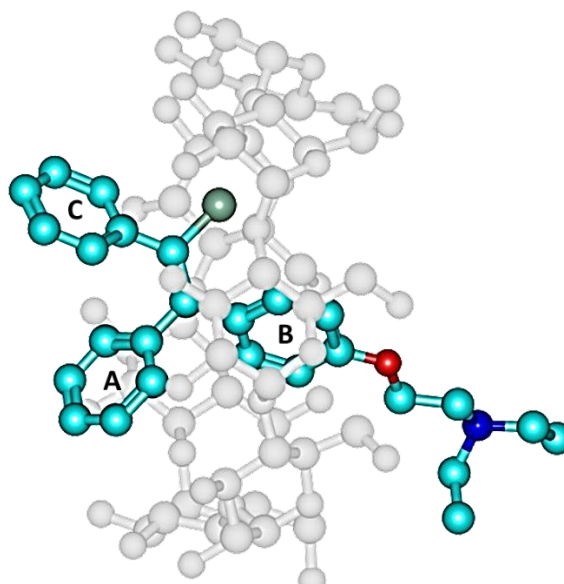


Figure S5. (Cont.)



(a) E-CL-AV



(b) Z-CL-AV

Figure S6. Structures of the inclusion complexes optimised in aqueous solution at the GFN2-xTB-ALPB level. The initial configurations were derived from MD trajectories and represent the “average” structures, specifically, those with binding free energies closest to the average values. The $\Delta G_i^{sol-OPT}$ was -1.867 kcal mol⁻¹ (E-CL-AV) and -2.606 kcal mol⁻¹ (Z-CL-AV).

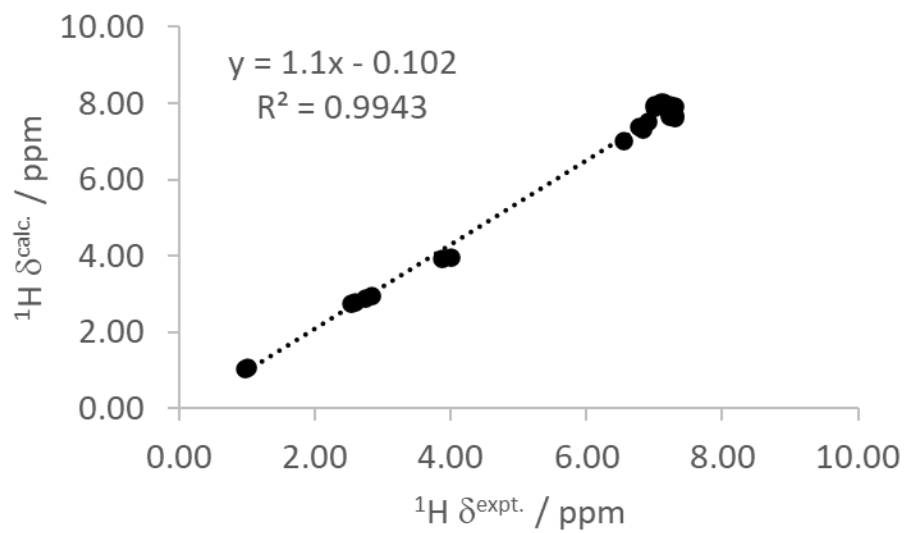


Figure S7. Correlation between the calculated and experimental chemical shifts for the *E*-CL and *Z*-CL isomers of clomiphen (CL).

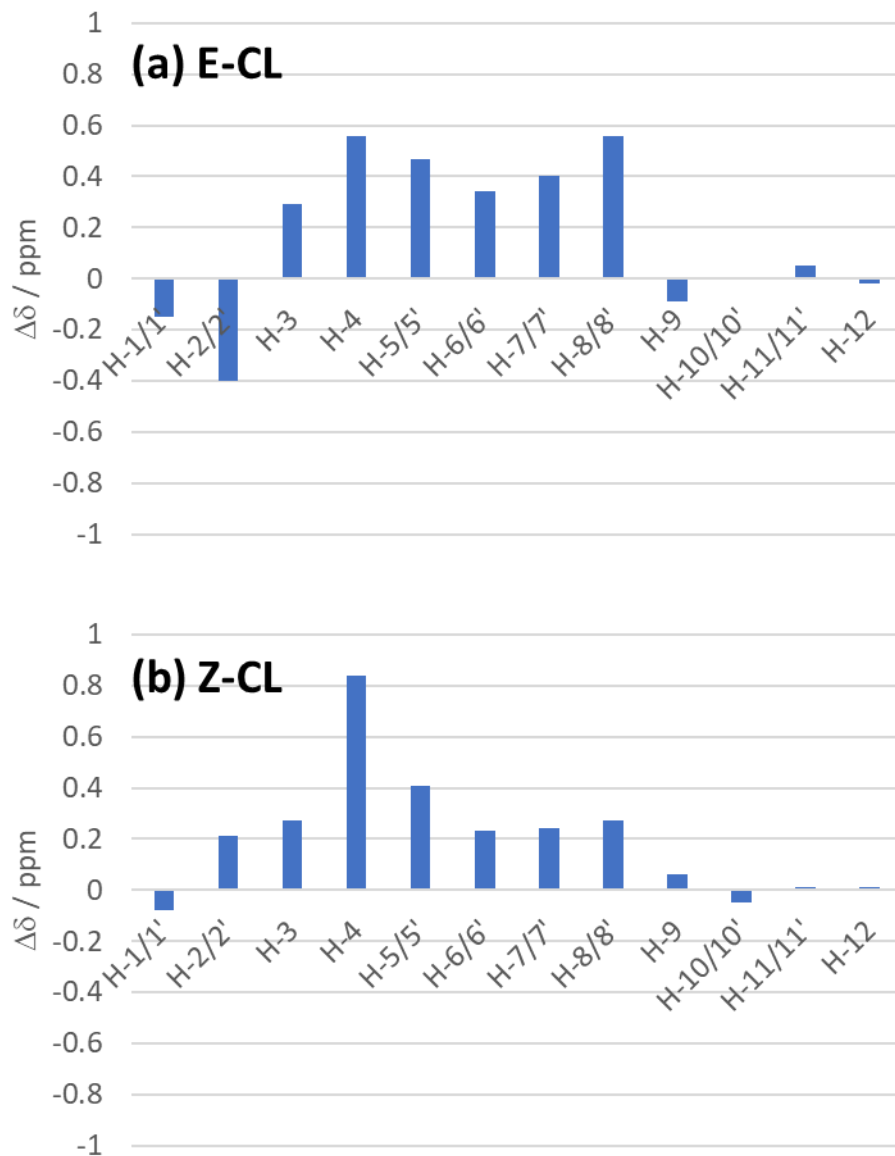


Figure S8. Variation of ^1H NMR chemical shifts upon the inclusion of clomiphen (CL) into the β -CD cavity.

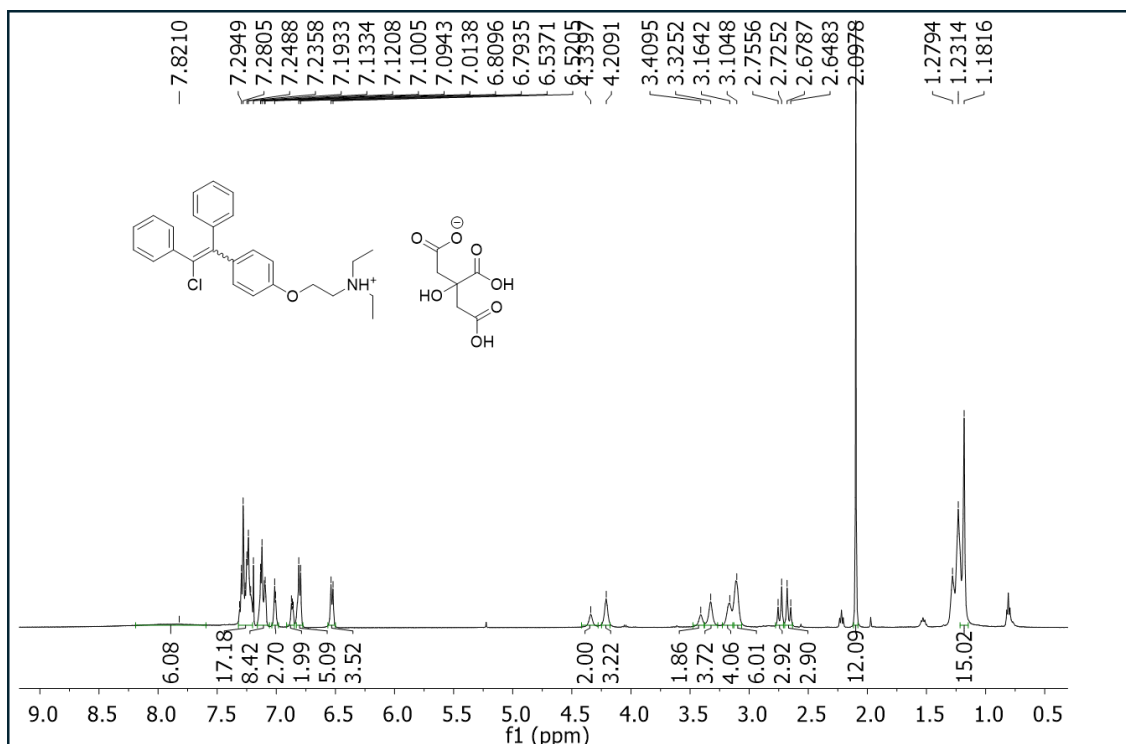


Figure S9. ^1H NMR spectrum (CDCl_3 , 500 MHz) of clomiphen citrate (CC).

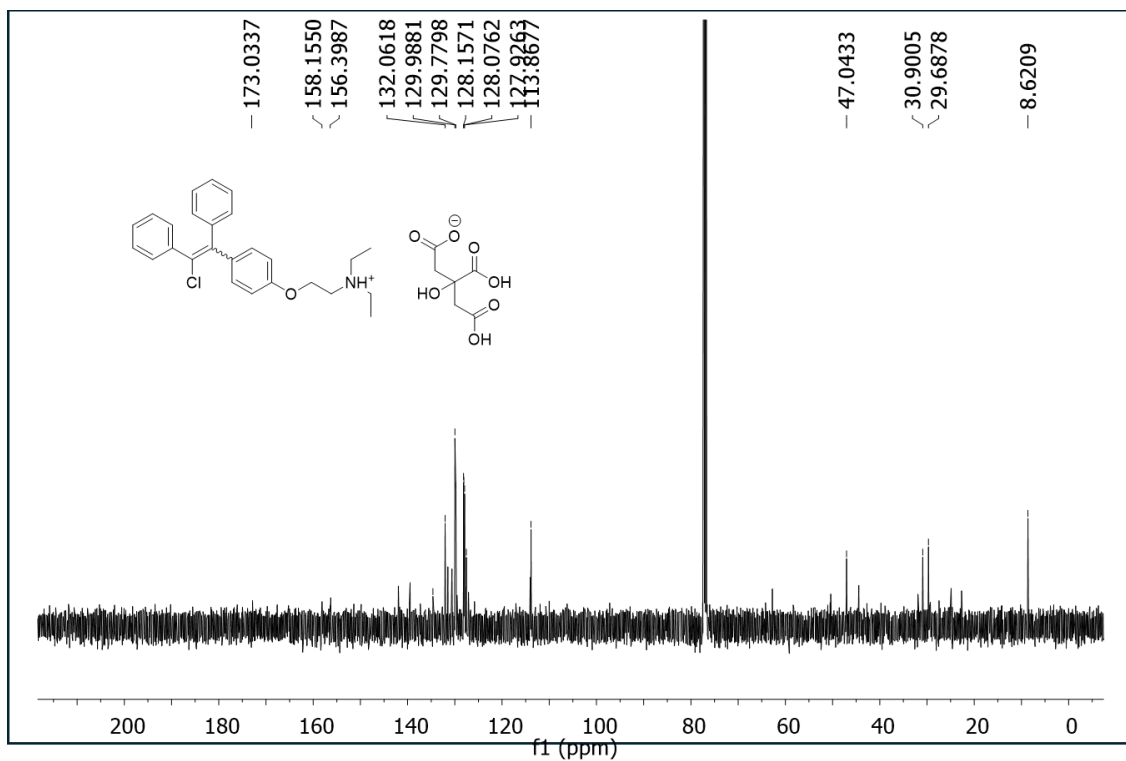


Figure S10. ^{13}C NMR spectrum (CDCl_3 , 500 MHz) of clomiphen citrate (CC).

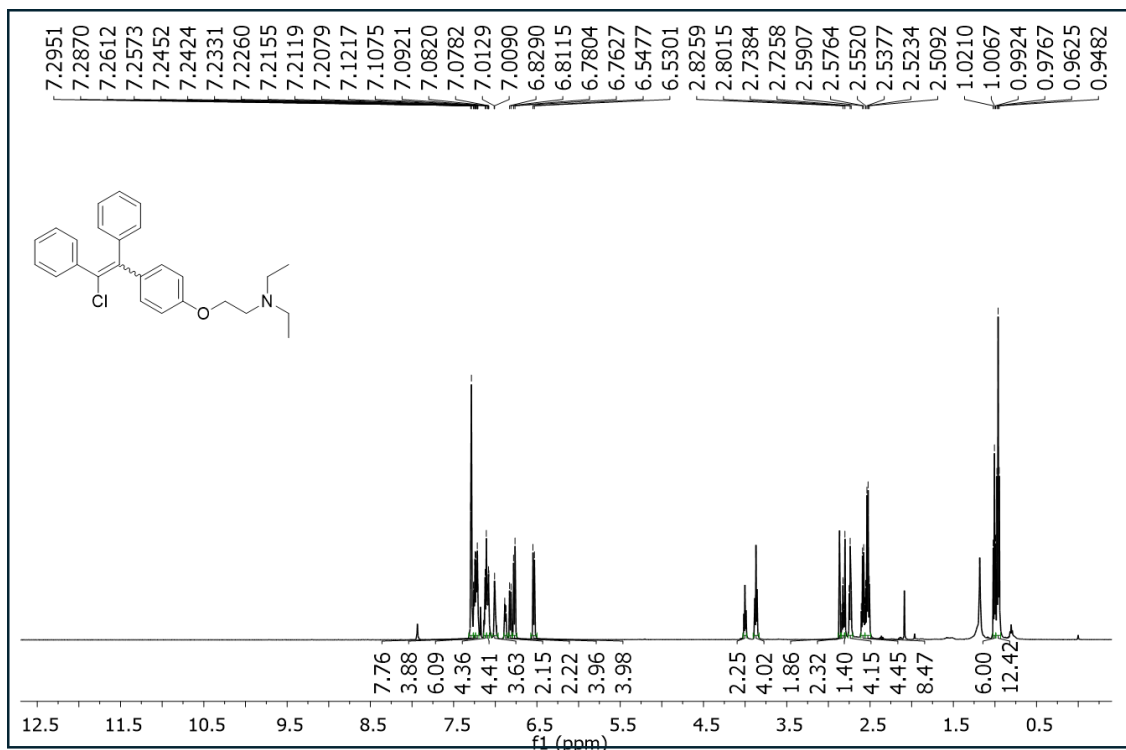


Figure S11. ¹H NMR spectrum (CDCl₃, 500 MHz) of clomiphenes (CL).

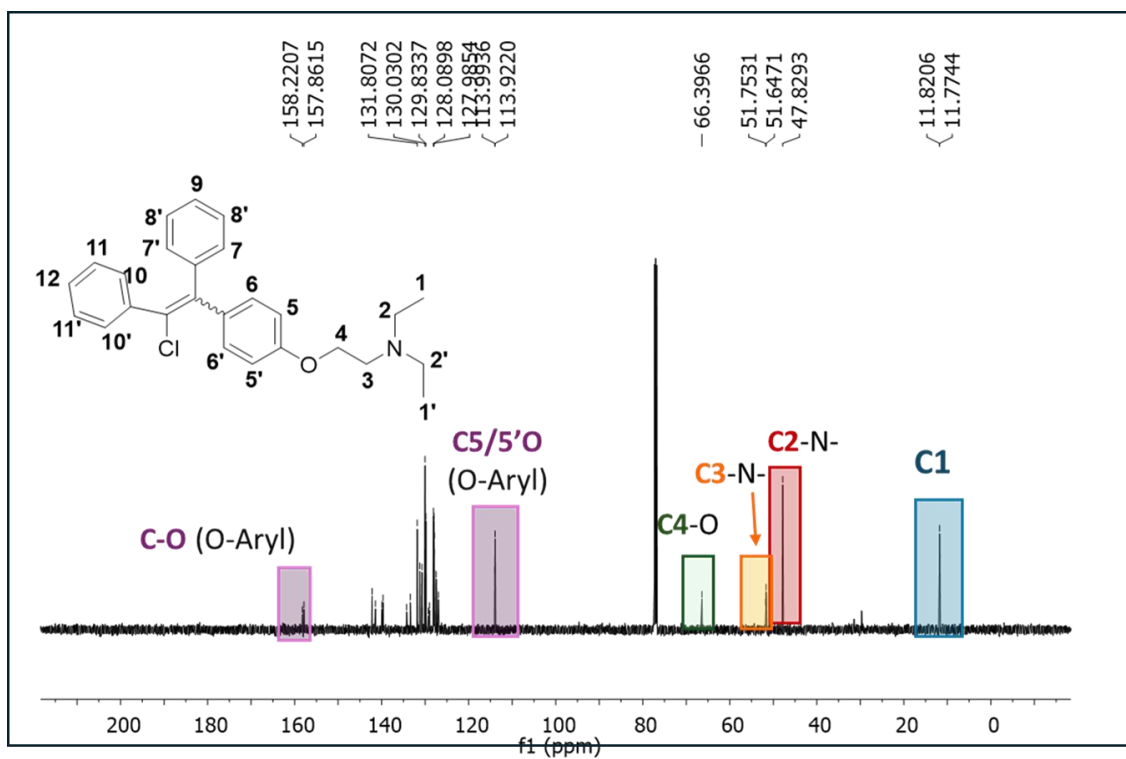


Figure S12. ¹³C NMR spectrum (CDCl₃, 500 MHz) of clomiphenes (CL).

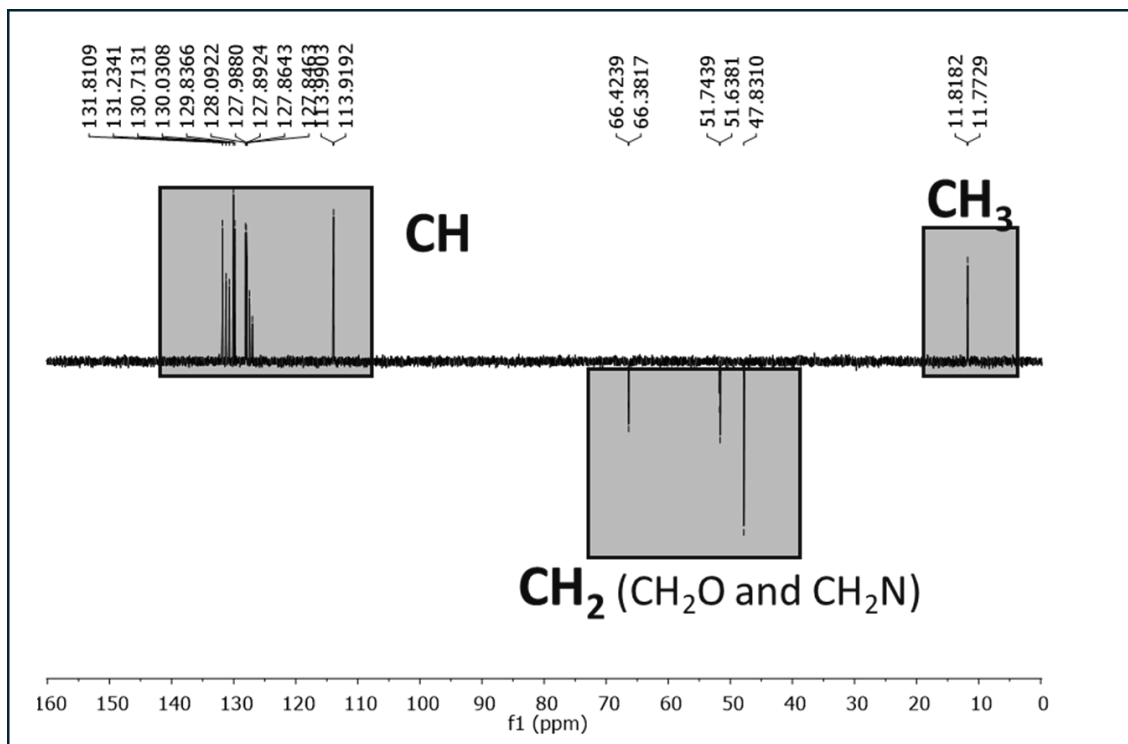


Figure S13. DEPT135 spectrum of clomiphen (CL).

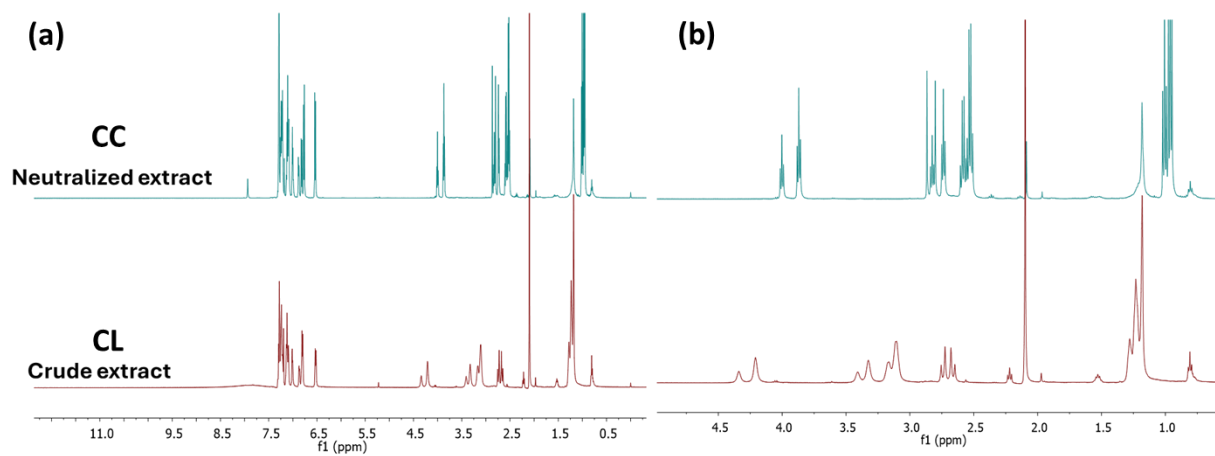


Figure S14. ¹H NMR spectra (CDCl₃, 500 MHz) of clomiphen citrate (CC) and clomiphen (CL): full (a) and expanded from 0 to 4.5 ppm (b).

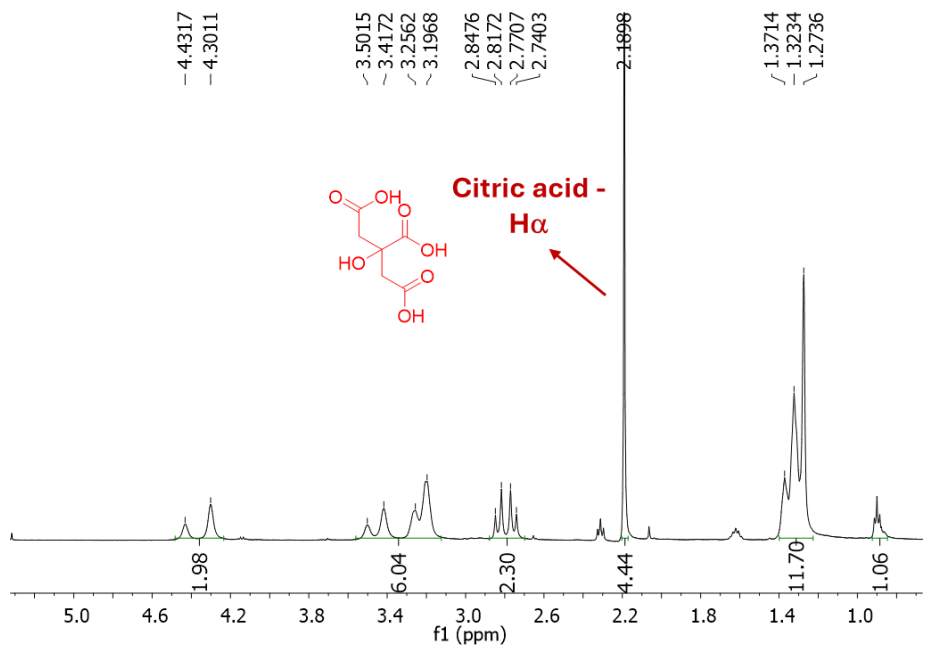


Figure S15. ^1H NMR spectra (CDCl_3 , 500 MHz) of clomiphene citrate (CC) expanded from 0 to 5.0 ppm.

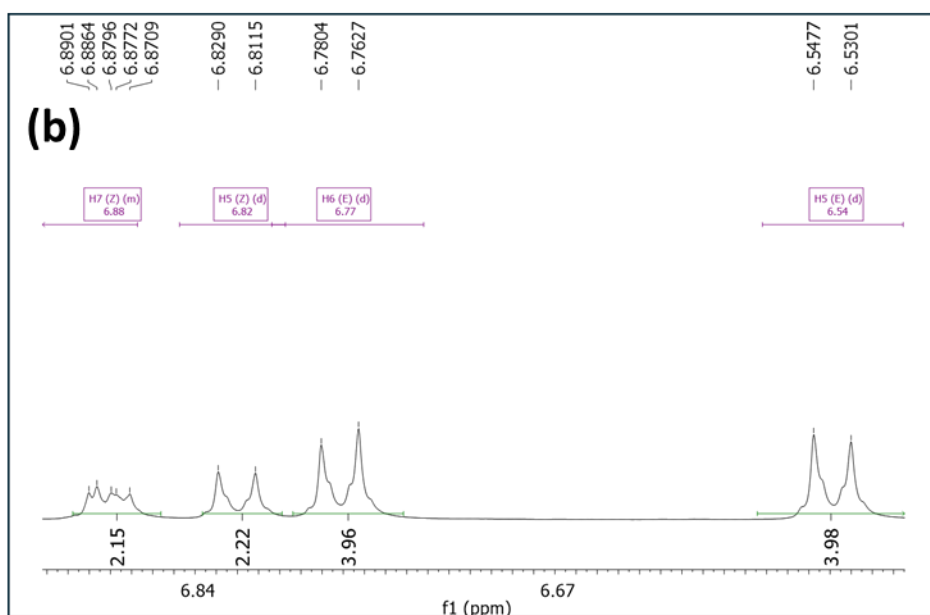
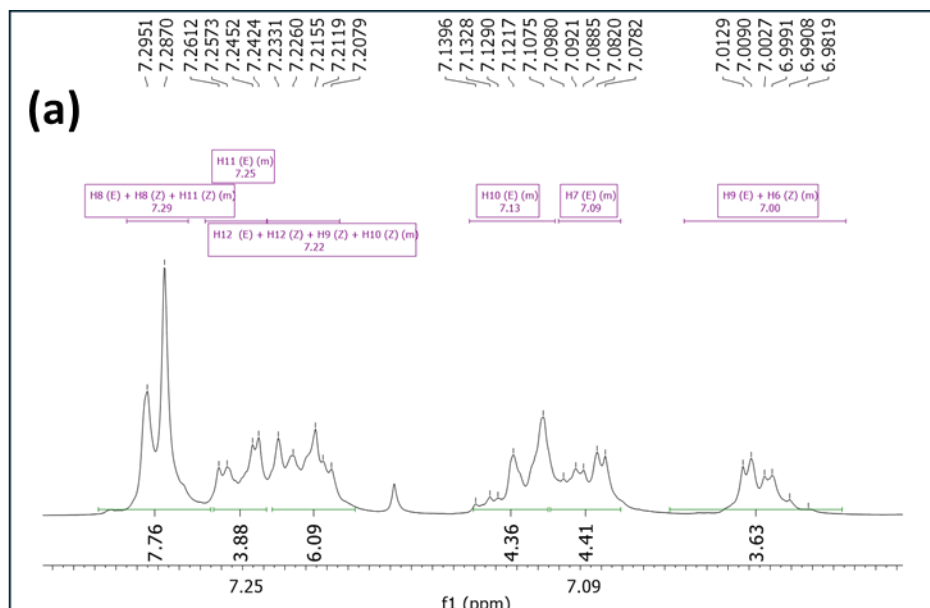


Figure S16. Expansion of ^1H NMR spectra of clomiphen (CL) of aromatic regions. (a) From 7.50 to 6.9. (b) From 6.9 to 6.3 ppm.

Table S1. GFN2-xTB-ALPB optimized geometries and total energies for selected structures modelled in the present study.

E-CL (Fig. 3a)

57	energy:	-81.474053022864	gnorm:	0.000496326152	xtb:	6.4.1 (afa7bdf)
C		3.98787638224412		3.69453867273136		1.41219898727096
C		3.70019365142339		2.35131831463236		1.25240823932706
C		2.90561177894495		1.92320989927937		0.19261846682528
C		2.39183765311502		2.86773587515254		-0.69256455565903
C		2.68818109240744		4.20875369930225		-0.53473198316456
C		3.48842044111921		4.62559228018806		0.51661141064778
H		4.60315150740464		4.01502004683049		2.23968173273170
H		4.07918835793862		1.62902462532800		1.96052610617250
H		1.76774391845206		2.53887521550361		-1.51055710644211
H		2.29262741482006		4.93140883378815		-1.23248960325746
H		3.71861267798668		5.67289950348641		0.64074419650987
C		2.57016991897337		0.49781341144824		0.01688869055136
C		3.4978409274934		-0.47189484360222		-0.02029634116397
C		3.24596425976836		-1.91401921326004		-0.04808943403349
C		3.96910974237640		-2.75393490931809		-0.89204326964073
C		2.29283517596109		-2.47013593149090		0.80586916856415
C		3.72617102548397		-4.11496608930753		-0.90145656747097
H		4.71558881013993		-2.33130204029103		-1.54822280940563
C		2.05760490549458		-3.83113742912572		0.79570081824929
H		1.74673175190253		-1.82780497880030		1.47920015168226
C		2.76906966549092		-4.65721629263142		-0.06025400823615
H		4.28749267073471		-4.75334750547647		-1.56683231114738
H		1.32001130594803		-4.25051335050625		1.46258714484174
H		2.58263441531116		-5.72011117822685		-0.06674089683703
C1		5.20221042057126		-0.05115147688557		-0.03196274637543
C		1.13865200195969		0.20410670271132		-0.16771023169638
C		0.19073984949079		0.84685798528163		0.62141433772129
C		0.69340710348121		-0.66998646697307		-1.16046455509734
C		-1.16230435280048		0.61057376345835		0.45698164152164
H		0.51711246757714		1.53498122960737		1.38710028058090
C		-0.65074055432663		-0.90484033083185		-1.33712829104093
H		1.41050395044874		-1.15375536724832		-1.80499935163657
C		-1.59682091347442		-0.27376772270815		-0.52479573585827
H		-1.86574958168470		1.12036829311233		1.09471080182184
H		-1.00199700895915		-1.57501084504328		-2.10537231037799
O		-2.89735505624077		-0.58416033430040		-0.77912168173097
C		-3.91416938693430		0.03843707282662		-0.01084441375636
H		-3.79684357632714		-0.20492007547095		1.05073723830747
H		-3.87415675044086		1.12642094123869		-0.13206317183687
C		-5.25809986675412		-0.49144665760409		-0.52296026508212
H		-5.26835343183831		-1.57914480190716		-0.39670902285833
H		-5.31272311600373		-0.29435078069132		-1.59889276961243
C		-7.19370927320875		0.96530557834658		-0.67502709212837
H		-7.55021832782956		0.41262841103416		-1.56331770145903
H		-8.07063902907048		1.26486998412628		-0.09714666110916
C		-6.45538910073201		2.22402582385191		-1.11761648421394
H		-6.09199342166644		2.76094870910731		-0.24632626769235
H		-5.61118253714660		1.98388692859511		-1.75783807031086
H		-7.13335733332075		2.86787754964438		-1.67143784726539
C		-7.13159156420466		-0.80624715167269		0.98931979103577
H		-7.47995797812478		-1.67008706447365		0.39430428280831
H		-8.01466009585309		-0.27952857900966		1.35743769421846
C		-6.33025260370776		-1.30004979139236		2.18899617303628
H		-5.47888252714448		-1.89873557663466		1.87765317927950
H		-5.96997174624233		-0.45102458166299		2.76245158968228
H		-6.96543582779760		-1.91149238709513		2.82426294634755
N		-6.36744846773453		0.13025134937369		0.18155084744359

Z-CL (Fig. 3b)

57	energy:	-81.474272555386	gnorm:	0.000641623623	xtb:	6.4.1 (afa7bdf)
C		3.77574480826336		2.91655493694731		1.41457228208746
C		3.39942025607688		1.60597896441010		1.18859900157050
C		2.52562071177477		1.29363971172035		0.14970938815510
C		2.02075644119213		2.32262323593316		-0.64151186749802
C		2.40496031310497		3.63190852839050		-0.41655103161660
C		3.28522280059569		3.93230099463629		0.60971553039142
H		4.45218015442292		3.14636383868726		2.22372015661299
H		3.77212143762778		0.81664387749492		1.82340758272802
H		1.33406754365103		2.08644739903259		-1.44122514476180
H		2.01445553022994		4.41986580161098		-1.04265292997352
H		3.58310391279758		4.95451218100666		0.78619368910298

C	2.08771511675083	-0.09543463785274	-0.09012606334734
C	2.96977440579505	-1.10756203335343	-0.08934735362511
C	4.42819608395777	-0.98161494208233	-0.04940452821860
C	5.19832646915580	-1.80428278275344	0.76970537077895
C	5.06914098627001	-0.04502507619166	-0.86132630359646
C	6.57452163529550	-1.67459858140590	0.79732095452493
H	4.70957694380403	-2.53846414453800	1.39294671721437
C	6.44472469945854	0.07725319880764	-0.83311144038723
H	4.48119754560377	0.57800169069291	-1.51742481000631
C	7.20156641082508	-0.73265403896246	-0.00101229505785
H	7.15840028732714	-2.31230449409827	1.44367934687599
H	6.92906312645719	0.80415811060311	-1.46698467595404
H	8.27599561081484	-0.63429642040645	0.02011516539015
C1	2.40205210841787	-2.76779473766411	-0.14363307352120
C	0.63889429215754	-0.27587083094026	-0.27733019485229
C	-0.25562441215017	0.34434112396645	0.58855724364724
C	0.12642448590359	-1.02488866478831	-1.33620870969413
C	-1.62240513681027	0.20740575369763	0.42974107728328
C	0.12560432002598	0.93488918053416	1.40833633620340
H	-1.23316597897392	-1.15770054246664	-1.50932531147284
H	0.80008948485685	-1.48778228441098	-2.04134823160001
C	-2.12545369883999	-0.54913987474544	-0.62389354075854
H	-2.28401031837674	0.69361688003105	1.12791836090205
H	-1.63591670565005	-1.73035471051498	-2.32991231907044
O	-3.44768743807822	-0.74906438486784	-0.88339116670527
C	-4.41044402287570	-0.14729793762077	-0.03334691878387
H	-4.29794895345286	-0.51339404301686	0.99305684551366
H	-4.29645106487240	0.94210838318026	-0.03639504753113
C	-5.79419323211635	-0.52751706474687	-0.57229703678878
H	-5.85953294773712	-1.62028867529611	-0.60111643511875
H	-5.86602100036876	-0.17590944583707	-1.60706434134935
C	-7.64591435617480	1.03784851830124	-0.44490308349414
H	-8.05695919985151	0.64413998450750	-1.39226200346027
H	-8.48825494418153	1.29495724803919	0.20081330415828
C	-6.84591152849535	2.30642899354362	-0.72098148396780
H	-6.42027020417770	2.67866166672240	0.20623705276718
H	-6.04071551429013	2.12162437759521	-1.42649767123386
H	-7.50088836086291	3.06587850607240	-1.13925472603895
C	-7.64720979622827	-0.96431651620259	0.93437365802070
H	-8.05664122351866	-1.71018695480273	0.22896993684865
H	-8.49070560648864	-0.45254828069256	1.40260659091060
C	-6.84966291393261	-1.67344616240158	2.02378077884120
H	-6.03871958346826	-2.26128503007466	1.60280245188064
H	-6.43155788850916	-0.94017496279755	2.70711066939494
H	-7.50425225807219	-2.34024199089846	2.57845472460559
N	-6.84902580494939	0.04053504754098	0.25100117198431

β -CD
147

energy:	-268.189926121588	gnorm:	0.000375802813	xtb:	6.4.1 (afa7bdf)
C	-6.16731266433820	-1.10983716176564	-0.15532144374737		
C	-6.59972142428232	-0.18132759444020	-1.30230807236510		
C	-5.63024757442317	1.00053340942018	-1.40813207777079		
C	-5.44573890242433	1.67472809590142	-0.03932278019325		
C	-5.07825568265998	0.62572094600295	1.02460885757940		
C	-5.01083726546845	1.20415464059598	2.43626749966297		
C	-2.96576154651392	-5.32112223380943	-0.14130883063444		
C	-3.88618605779574	-5.16676407816840	-1.36303916304924		
C	-4.23848768089496	-3.69162638415408	-1.56786889742657		
C	-4.78364518688900	-3.09590125631347	-0.26003048807195		
C	-3.79070551813668	-3.35050448927334	0.88667282865966		
C	-4.28619278937577	-2.86748284048210	2.26112297174546		
C	2.29223177934445	-5.48781285308176	0.27813188772701		
C	1.63538321735877	-6.27680478841271	-0.86736442855301		
C	0.32396991200086	-5.59663174058584	-1.26238811652525		
C	-0.56152095870489	-5.44358635370112	-0.01835946613171		
C	0.19718109719310	-4.69159348147545	1.08695518612122		
C	-0.57857668921199	-4.61103124544212	2.42143056151147		
C	5.89902066462512	-1.62692355411395	-0.09758218555549		
C	5.90814958803861	-2.65959949686133	-1.23545239859584		
C	4.52520610472528	-3.30277108369563	-1.37483900647471		
C	4.03645147308188	-3.82382703480522	-0.01416763859308		
C	4.13973514536469	-2.71402030446436	1.04641908258459		
C	3.78054615188885	-3.19827057885093	2.44971412905823		
C	4.93611173019340	3.56096219876183	-0.14492085536229		
C	5.71656693151599	2.99915262510745	-1.34261245157956		
C	5.35936615957652	1.52534046213370	-1.54200142205727		
C	5.54732957592451	0.76015341277060	-0.22397488868840		
C	4.76197552896722	1.44193369497976	0.90760325600237		

C	4.97211645507418	0.79015982579819	2.29112361463792
C	0.25964974578397	5.99305476818522	0.13789520414110
C	1.16991555738989	6.37107884161951	-1.04058306925355
C	2.09702815885099	5.20086459177217	-1.37546010934892
C	2.82811389616250	4.73941455421721	-0.10573129956034
C	1.81184802184003	4.42547707561971	1.00358892617363
C	2.45718272696625	4.01415170345916	2.34463837163389
C	-4.59005641030105	3.91603788523247	0.32333885263381
C	-4.31739917106290	4.95713803795188	-0.77677517803562
C	-2.83165322118985	4.95004937198781	-1.14486235868824
C	-1.98225775617599	5.09923410534727	0.12558534298249
C	-2.36790575092224	4.00924331375358	1.13804260924133
C	-1.60796029609763	4.09755811903243	2.47814662006232
O	-6.62950243041336	-0.94218906266273	-2.47964974814745
O	-6.15976496434873	1.89389275053947	-2.35450051109150
O	-4.41776838430554	2.63529805613807	-0.22061334932817
O	-6.06836022441491	-0.40050254899429	1.04790916930785
O	-4.30084239564890	0.30575744946000	3.26371743101920
O	-3.21985514814960	-5.71078726606475	-2.46969369045138
O	-5.18646620288390	-3.62073052272374	-2.60298264277124
O	-4.95542247297244	-1.70948585685274	-0.50853021419762
O	-3.54249169892683	-4.75181190676115	1.00338354207624
O	-3.21983150743211	-2.38007964632098	3.04260413578574
O	2.54006463265198	-6.33497169410617	-1.93768189060934
O	-0.28871255048705	-6.39383610484629	-2.24467755109776
O	-1.72680309384546	-4.74534536616824	-0.43441011465783
O	1.42742503293968	-5.36282649681390	1.36936512795609
O	-1.35818762149403	-5.74953838478452	2.69288347345701
O	6.29901878500090	-1.99817138565440	-2.40847257524698
O	4.64386563040195	-4.33637232245295	-2.31884833378435
O	2.69177495102087	-4.23389097551645	-0.20906446472571
O	5.47316532302042	-2.21111838094752	1.10465713172050
O	3.53385038564383	-2.06704574364699	3.25349540988233
O	5.39601765194627	3.77956532137772	-2.46260155049354
O	6.18998103450190	1.01982735876674	-2.55663779000869
O	5.08093942181901	-0.55830194015957	-0.47090434586649
O	5.16444124712474	2.80920329984585	1.01724917255933
O	6.27481505781426	0.29604706931127	2.49051592716407
O	0.34448265035300	6.71919491050820	-2.11880556685745
O	2.99731258096667	5.64144728690296	-2.36046724176068
O	3.57764464322258	3.59075413217016	-0.47481886733060
O	1.00505419932757	5.57744850718408	1.25231955796464
O	3.63809446266412	4.70772472409950	2.65256230280018
O	-5.12974632322675	4.64347023922318	-1.87662428235714
O	-2.61568715591461	6.00791018986163	-2.04476168404797
O	-0.62591428027404	4.99704122946867	-0.28410180259582
O	-3.76110062006237	4.11472994147261	1.43255891606427
O	-1.38219888934029	5.40641983620763	2.93229690106362
H	-6.94513270570626	-1.86531815904467	0.01708652925638
H	-7.59958051809884	0.21327902241025	-1.06939571117167
H	-4.64818796741331	0.62650343324320	-1.73583211703323
H	-6.38556364588423	2.16616719406702	0.24537226758789
H	-4.10587309748004	0.18703505158081	0.76473270134068
H	-4.50169444242523	2.17416342592867	2.40441962050292
H	-6.03790163099378	1.33305035139055	2.79295382624244
H	-2.85590244134178	-6.38924065885998	0.08820423035773
H	-4.81718678988531	-5.71714517753918	-1.16148026601179
H	-3.32555574553416	-3.14037125892713	-1.83966523228844
H	-5.74584235466944	-3.56759773035806	-0.02182274971557
H	-2.85018380021856	-2.83765265284569	0.64279640709484
H	-5.05283423571162	-2.10313004292606	2.13290035732574
H	3.15541024350001	-6.04940204154506	0.65808541161148
H	1.40542850270549	-7.28744353134305	-0.49975210068750
H	0.54241721998790	-4.59341569029588	-1.65828840596744
H	-0.82318573933411	-6.44121031308902	0.35782042770164
H	0.42158473289227	-3.67590837815875	0.73533736448255
H	-1.19447883212696	-3.70909795186869	2.43683289445800
H	0.16897705524068	-4.54801848618185	3.21590160214126
H	6.92684547533063	-1.28815200177708	0.08623557717372
H	6.62866936498508	-3.44953235789463	-0.97696897294289
H	3.80940516603753	-2.54156723478701	-1.72124738254559
H	4.65944118390924	-4.67616372651353	0.28714253176543
H	3.45811881576110	-1.90020336808259	0.76546050274307
H	2.88933445017801	-3.83402350070899	2.39053161424319
H	4.62544905898420	-3.77890283381495	2.83691054248621
H	5.30694223909461	4.56967123121744	0.07994496947969
H	6.79050369559650	3.06642462320198	-1.11504529316909
H	4.30094493887583	1.44893985669010	-1.83453090844392
H	6.61257334467589	0.75298464104298	0.04084647853479

H	3.69413159663916	1.40912188710689	0.65218179042367
H	4.80965475765567	1.56919828033317	3.04178901918059
H	4.23459862738594	-0.00227507478139	2.43213832619878
H	-0.28515097964278	6.88778802367084	0.46684933701976
H	1.79135520116217	7.22521692060498	-0.73387117628444
H	1.49366418800493	4.36005571079581	-1.74995431584002
H	3.49139247206323	5.54318403674153	0.23906864137482
H	1.16312720981271	3.61022868058837	0.65485123693779
H	1.74210140539351	4.25489045621074	3.13595921395772
H	2.63163225996158	2.93508461416572	2.33357263273339
H	-5.61320581997905	4.04499524093857	0.69879683974359
H	-4.56852636830711	5.95148398044378	-0.37986802892302
H	-2.58116632032579	3.98642483363217	-1.61388985125228
H	-2.17846125784729	6.08113918974023	0.57553564190907
H	-2.17751151855981	3.02543677030859	0.68847857706999
H	-0.66695493209578	3.54973823931432	2.38384361026855
H	-2.23350262726731	3.61240656111985	3.23092104188452
H	-4.71994446533080	-3.73015160872280	2.77660677979110
H	-6.81711894818551	-0.34164365646456	-3.21882121789928
H	-5.72453750352441	2.76190561141321	-2.26533017195177
H	-4.43103375106152	0.56508264111314	4.18697076500275
H	-3.75617130770200	-5.53338263531639	-3.25907294257193
H	-5.56805592145597	-2.72487732360252	-2.63360541972652
H	-3.29768673352901	-1.41433041490901	3.11180792723899
H	2.08136627678426	-6.74614814223138	-2.68862711398665
H	-1.20069459689026	-6.08564635693583	-2.39412818335845
H	-2.26138569188279	-5.58682150633765	2.37745625267385
H	6.22390790955040	-2.62625027505469	-3.14469134702149
H	3.87462282111165	-4.93279319366340	-2.25465572080944
H	3.40318184183306	-2.34593915207671	4.17091432316812
H	5.80949534928609	3.37113374967703	-3.24012868442637
H	6.13301115274646	0.04730430338892	-2.57167358475039
H	6.26769513473858	-0.66012034230573	2.33299410236959
H	0.91171375528062	6.87157250981216	-2.89158770404423
H	3.70728208838380	4.98402758301228	-2.47207587523148
H	4.39629919013029	4.21582240555926	2.29808452766242
H	-4.89262566078061	5.24601665835278	-2.59979136098318
H	-1.65893468015262	6.14846808489992	-2.16047350706369
H	-0.53509068901449	5.72270737148106	2.57857995626286

E-CL-6 (Fig. 4a)
204

	energy:	-349.686931048418	gnorm:	0.000227978935	xtb:	6.4.1 (afa7bdf)
C		-1.26712203851834	-0.66137134352397	1.31643908331152		
C		-1.18693860873413	-0.43020216409576	-0.04455574099211		
C		0.04614257092704	-0.18980360733958	-0.64779022906399		
C		1.20038339998080	-0.25447048437613	0.13318189842681		
C		1.11785896227130	-0.49831896534941	1.49192766026406		
C		-0.11790974133040	-0.68587321095153	2.08938830122476		
C		0.16302792224920	0.16589244075048	-2.06959073122968		
C		-0.61510340208128	1.07177866389184	-2.68132348952443		
C		-0.54841444345397	1.42659853984286	-4.10302446261193		
C		-0.54750796324766	0.43133867488493	-5.07926369649337		
C		-0.51750264011422	2.76233789849740	-4.49731372139789		
C		-0.51041500183637	0.77053666306214	-6.41885307893587		
C		-0.46201778160981	3.09589871084623	-5.83748077018041		
C		-0.46029781959650	2.10135219980039	-6.80159171812419		
C		1.29871598841381	-0.42323100467693	-2.80768075526139		
C		2.24423733655371	0.40093408383413	-3.40562340165717		
C		1.46949416350461	-1.80246521672618	-2.88836454230441		
C		3.33030145590491	-0.12508465299302	-4.07721119564298		
C		2.53137353628870	-2.33540065283867	-3.58705028762597		
C		3.47970710974163	-1.50344551429680	-4.19152953909886		
O		4.50565939950096	-2.14126972819899	-4.81627954412644		
C		5.32738827803720	-1.46669385450215	-5.75988170761932		
C		4.83735474021592	-1.63901796047820	-7.22049781837442		
C		2.37988495944923	-1.57226047934497	-7.22344466863472		
C		1.59416537524435	-2.07788392416797	-8.43480105677668		
C		3.66954718982181	0.48953421796220	-7.55266448015217		
C		2.86802338269395	1.13245061455973	-8.68217256118859		
N		3.63476916168753	-0.95704759103010	-7.62545416267221		
Cl		-1.82185741348860	1.98526693783066	-1.78627115401490		
C		-6.03627812133331	-0.91428542206077	-0.77697999971762		
C		-6.42826508657655	0.11014554840922	-1.85587000339671		
C		-5.54197622344767	1.35608390176841	-1.76362206842185		
C		-5.45378375379181	1.87524102716255	-0.31960978011579		
C		-5.09211340957877	0.72632064327070	0.63777884523116		
C		-5.10570046984746	1.14081455585890	2.10692649642618		
C		-2.76779722446999	-5.06155827179106	-0.75223278152941		

C	-3.38974012768587	-4.73657317043914	-2.11914097933000
C	-3.73314250900467	-3.24732397177152	-2.18863139308573
C	-4.61095947670491	-2.86108963922815	-0.98933511117851
C	-3.92624464827305	-3.27634869633070	0.32548816276252
C	-4.80464152485825	-3.06797227222101	1.57527019571053
C	2.307181375257576	-5.38931286551439	0.58274750859687
C	1.74302849183474	-6.27149304787163	-0.54378598828602
C	0.55586349877074	-5.54667871096963	-1.17878595808430
C	-0.46810159871497	-5.22131123071002	-0.08176238998257
C	0.18001685762751	-4.44642683490052	1.07484623379181
C	-0.77806051637024	-4.28695253998232	2.27779291320193
C	5.99468230247822	-1.63507729864793	-0.01053863724810
C	6.01393978102394	-2.72891130289516	-1.08934071449042
C	4.64084338247679	-3.39546127101049	-1.17504622803203
C	4.14275271168572	-3.83352072320853	0.20910290515905
C	4.26373515818555	-2.67283071962269	1.21026892545586
C	3.91301465469269	-3.09384055380050	2.63551971066337
C	4.87036413790140	3.50729002760117	-0.28348588381782
C	5.59623131438668	2.91441826473348	-1.50078875587079
C	5.27041059423460	1.42328708455701	-1.61070347197871
C	5.57349475208260	0.72963968813511	-0.27614695517501
C	4.83491103875778	1.43390384689718	0.87221116045579
C	5.15644523918647	0.85582043606532	2.26534387819379
C	0.24395991970709	5.98281047370375	0.22375848516785
C	1.14991415730562	6.36248885451302	-0.95773406554657
C	2.01381891976558	5.16472541957577	-1.36358900284082
C	2.74569485484305	4.62979855289606	-0.12243505537604
C	1.72442110876464	4.28673003973047	0.97313496046062
C	2.36004665813515	3.76749413477708	2.27969090098908
C	-4.66834837272899	4.07495384287214	0.35974968933812
C	-4.42199573023268	5.26486336002576	-0.58359372070280
C	-2.94679449144248	5.30319252000930	-0.98589090218351
C	-2.04598974199579	5.22830220013422	0.25650658781917
C	-2.44753079726101	4.05777875043744	1.16641493764234
C	-1.67376451443178	4.01564285185224	2.50203352661189
O	-6.31482289850924	-0.52149189013270	-3.10148854635398
O	-6.09712552173333	2.32406235888551	-2.61780011879959
O	-4.46175573588143	2.88893221925330	-0.35616217283365
O	-6.04379665681401	-0.32402682188104	0.49331491542700
O	-4.404422987119222	0.17502626077511	2.86326994210521
O	-2.47628954137896	-5.11815183660157	-3.11042566513495
O	-4.39466470138241	-3.01962750990671	-3.40685403855094
O	-4.78665408276086	-1.45493180363357	-1.09300978383621
O	-3.61017453893959	-4.66896439767973	0.29724144964094
O	-4.04756529474806	-2.68677931766469	2.69649586782389
O	2.76743341224204	-6.51266897357849	-1.47146065507689
O	0.01905377432573	-6.39179888217656	-2.16605992552173
O	-1.51281814840166	-4.45034260774131	-0.66246488671536
O	1.33562357884618	-5.13407063419005	1.55509375925751
O	-1.62253820883349	-5.39029784488615	2.48284838818222
O	6.36939053429299	-2.12602992929270	-2.30721646371315
O	4.75628006768005	-4.48189775109549	-2.05816406848087
O	2.78480690166941	-4.19724320458584	0.01890914077491
O	5.59410202415585	-2.15903491653420	1.22702891109223
O	3.69523411633204	-1.93384005110288	3.40640788607220
O	5.18684523972955	3.64113596264931	-2.62736116537534
O	6.03377161676062	0.87604588633963	-2.65759845430462
O	5.14481477119022	-0.61269619350303	-0.44071216589139
O	5.18962812544046	2.81802005226372	0.89506051862889
O	6.50169627259888	0.46604661483266	2.41152661368564
O	0.32330952640981	6.80417481336616	-1.99969341672400
O	2.91213951922562	5.60953151545181	-2.34687298335384
O	3.49242413738131	3.49328540278549	-0.53065802456199
O	0.97925375586099	5.46013516979363	1.29906598006177
O	3.53682549737596	4.43157326956988	2.65277043956479
O	-5.26244982128710	5.11005388300782	-1.69581182470762
O	-2.73092862664955	6.49573090170716	-1.69854450642691
O	-0.71829127063468	5.07592729223630	-0.22722222684258
O	-3.83603844311136	4.14326009266898	1.48304397324040
O	-1.36013896682464	5.27422235634265	3.03522519666923
H	-6.80127161019313	-1.70125825179507	-0.73774712985371
H	-7.46637210066640	0.42061126504162	-1.66621327597127
H	-4.52300464354287	1.09460087307358	-2.08777143896494
H	-6.42467397592655	2.29866385204982	-0.02946086667000
H	-4.09288257090046	0.35388013259946	0.37846891422134
H	-4.62522610191150	2.12030805501756	2.20574825205690
H	-6.15092707698533	1.20048602659646	2.42958751282145
H	-2.68079763682135	-6.15132373312252	-0.65077166964486
H	-4.32470596785925	-5.30908287324184	-2.21438590636150

H	-2.80185006612726	-2.66176875182938	-2.13757828456710
H	-5.57960115493682	-3.37195906331347	-1.07513319369848
H	-2.99779998806367	-2.69777106630286	0.42245004305493
H	-5.58049008444599	-2.33009559257272	1.36884294058995
H	3.10880427213173	-5.92766718646778	1.10424125138394
H	1.38904733936712	-7.21442541988620	-0.10346802655047
H	0.91111581570940	-4.60516916726884	-1.62105564492249
H	-0.86102390235383	-6.16602115704031	0.31627008532903
H	0.47959165996172	-3.45265043662229	0.71516019984173
H	-1.35886050206799	-3.37037097739188	2.15606261566961
H	-0.15495417265539	-4.20174334527362	3.17103796308058
H	7.01473231721643	-1.25921963969526	0.14123274057945
H	6.75697203271042	-3.48925014633856	-0.80556106930448
H	3.91904812929132	-2.65955703739150	-1.56364891363063
H	4.73220885776572	-4.69174605409471	0.55712644373006
H	3.57393242362893	-1.88244590735363	0.88924384295297
H	3.00561104095166	-3.70927732174187	2.60423485057588
H	4.74878256975253	-3.67885541729305	3.03492366401526
H	5.22787393850522	4.53324739511400	-0.12294128946027
H	6.67825768013791	3.02286765533818	-1.33799760940277
H	4.19644134154664	1.30493351333782	-1.82209433387336
H	6.65307128374275	0.77233075891499	-0.07964662183710
H	3.75520298440066	1.35068549464246	0.68848292197642
H	4.96688501013226	1.64841609364133	2.99578052867770
H	4.48874826127232	0.01731953399739	2.46800481586936
H	-0.23118120639476	6.89322309627627	0.61307984223531
H	1.82135593857261	7.16841175957524	-0.62654345482617
H	1.36692595954430	4.36584055531171	-1.75825817978015
H	3.41264886716352	5.41403368184766	0.25943950797328
H	1.03686561180179	3.52164366308555	0.58458225964342
H	1.64195228901682	3.94316836752100	3.08483633400547
H	2.52799769332537	2.69102716999693	2.18069592870281
H	-5.69344179460020	4.12376685226131	0.74841950175994
H	-4.65759465560725	6.18994220925365	-0.03843375140479
H	-2.73037531284836	4.43284299841833	-1.62073407418076
H	-2.1505249503900	6.16330765970561	0.82266988451115
H	-2.26782723634238	3.11608252431422	0.63148339442519
H	-0.77252645820791	3.41185486136473	2.36389523703390
H	-2.32614479235368	3.52633490442219	3.22870408479404
H	-5.27164278421032	-4.02939409765469	1.80726757489667
H	-6.52160045799589	0.12961081853554	-3.79090183560379
H	-5.72409449501343	3.19865534393351	-2.40832854820389
H	-4.49536966185677	0.39502753255737	3.80201684208006
H	-2.80812886515327	-4.79713902905003	-3.96458227306984
H	-4.85113518392405	-2.16187235742769	-3.37318703652212
H	-4.07658547216256	-1.71702723583317	2.77723747238656
H	2.37977494053179	-6.99821569196253	-2.21805901789290
H	-0.75164254350118	-5.96369311652942	-2.58058862043701
H	-2.44435755920341	-5.26104303574020	1.98267813818021
H	6.14622581402310	-2.75125582797145	-3.01566639203021
H	4.03169493088713	-5.11561278843686	-1.89589485224250
H	3.61213922618452	-2.18052044065682	4.33874262859811
H	5.64498221435387	3.28159029942031	-3.40261324016854
H	6.07736635652127	-0.09144439126098	-2.54696472079768
H	6.54982983599727	-0.49942197215580	2.36082798185156
H	0.89003464349802	7.01696508376313	-2.75863467445327
H	3.58186507141531	4.92298694537500	-2.51685133220566
H	4.29359098795371	4.02354440935416	2.19771873863496
H	-5.07147960906155	5.83060054884185	-2.31813691714333
H	-1.78209979579418	6.58917530594792	-1.89481242301297
H	-0.50449023892932	5.56716646962544	2.68006137593596
H	-0.42620066249992	4.13395741230419	-6.12962878439560
H	-0.52700789377161	3.53533107632478	-3.74245156189019
H	-0.58994275762788	-0.60482218722839	-4.78048334023706
H	-0.52972780691672	-0.00743520119561	-7.16684747804256
H	-0.42727332091474	2.36416583897724	-7.84760588328667
H	-2.08421475228586	-0.44619481512888	-0.64800191108575
H	-2.22949174102718	-0.80831878086770	1.78312884477531
H	-0.18655018824878	-0.85932858214467	3.15120002564305
H	2.01459241943901	-0.53858700585076	2.09244207230712
H	2.16213675030982	-0.09529200799326	-0.33640905537444
H	2.13560035027753	1.47275857556735	-3.32705081299779
H	0.74839900407094	-2.45376105289297	-2.41486020646381
H	2.66149895552161	-3.40273780354021	-3.67467858568516
H	4.06339968032027	0.55158227651909	-4.48233875511851
H	6.30340724219861	-1.95036053846153	-5.67759435621660
H	5.44578445035965	-0.41197521206483	-5.51056047276513
H	4.71268776788463	0.80154739059143	-7.64224675013545
H	3.27609652155401	0.86290724071431	-6.59189844288561

H	3.18510708926635	0.72837266480420	-9.63900429733266
H	1.80650184124708	0.94593760997387	-8.55186598211055
H	3.02975152546765	2.20722087703619	-8.67923986485497
H	5.65227109821530	-1.29235895582044	-7.86315348310093
H	4.69174842818728	-2.70554132597033	-7.40430696750673
H	1.77196213520124	-0.85614084171513	-6.65609874506497
H	2.57522770965124	-2.42375490304832	-6.56618955036965
H	2.19321928975800	-2.79457576886938	-8.98958209955224
H	0.68028554776102	-2.56567204366942	-8.10495771991534
H	1.33880386058878	-1.26054474312366	-9.10127030818531

Z-CL-6 (Fig. 4b)
204

	energy:	-349.690561747151	gnorm:	0.000355205341	xtb:	6.4.1 (afa7bdf)
C		-3.38964648200078	-0.51770100754398	-4.50263448950134		
C		-2.43907201769291	0.15287395553532	-3.75417219327436		
C		-1.49474863925233	-0.56009651932758	-3.02347225818312		
C		-1.52522370099460	-1.95056904895148	-3.04236700322192		
C		-2.45370591619018	-2.61792495368596	-3.82064988223465		
C		-3.39034294323310	-1.90230060628301	-4.54908143656591		
C		-0.45312375164309	0.12718772042415	-2.23157607189735		
C		0.37763841964664	1.00227768797802	-2.80812820091123		
C		0.40539084314566	1.34571278698018	-4.23345599639853		
C		0.40177942994587	2.67867496847812	-4.63685632919807		
C		0.43768774342109	0.34326049144294	-5.20131657485146		
C		0.41166016398320	3.00245423647655	-5.98081357420654		
C		0.45213632492947	0.67212666004523	-6.54360688462838		
C		0.43589649400471	2.00055396427570	-6.93701840791593		
C		-0.43501495284438	-0.17167659247494	-0.78897649025816		
C		-1.58740282651710	0.05984896758399	-0.04036381048555		
C		0.69402800477882	-0.65495329108513	-0.14041621309512		
C		-1.60401349202488	-0.16286210214244	1.31904337099349		
C		0.68262114155905	-0.90147980553056	1.22117308512074		
C		-0.46741243115058	-0.65567007608956	1.96720481896177		
O		-0.59506545586043	-0.87546043563018	3.30499535043005		
C		0.56183058112601	-1.22391925766685	4.05250879957513		
C		1.54638975636691	-0.05842818292726	4.22927322598487		
C		2.50775553027326	1.49080582904377	5.81207938352940		
C		3.74761812634421	0.70457784135378	6.22999195853617		
C		0.09224317837034	1.26748497470262	5.67239857389240		
C		-0.17114350891101	2.49422782847398	4.79164459098377		
N		1.38293587565350	0.61837003997923	5.50250509254407		
Cl		1.55431844959772	1.87297421772437	-1.82745404102518		
C		-6.33670543444979	-1.07653750678515	-0.35242901601536		
C		-6.69992747522950	-0.33943356556354	-1.65322086302071		
C		-5.67212779905819	0.76787404639317	-1.90123016249275		
C		-5.55790383340747	1.67532445042107	-0.66614390950480		
C		-5.32211762473733	0.82871813131042	0.59787131333416		
C		-5.35630238192391	1.62319351326343	1.90273654012876		
C		-3.08854098767904	-5.24697760248744	0.08256877053327		
C		-4.14328478413380	-5.25739565437498	-1.03324474228990		
C		-4.53922774495382	-3.82296000074002	-1.38434569750165		
C		-4.94516848497642	-3.05045255201920	-0.11825440077339		
C		-3.86078583327429	-3.18263256150081	0.96691457926318		
C		-4.31576722736986	-2.60526463255614	2.31671099692638		
C		2.17372715715956	-5.42666132435663	-0.08803476617162		
C		1.41894169394292	-6.16462501808311	-1.20759802541049		
C		0.06767619117416	-5.49070447834244	-1.45600267002021		
C		-0.69219982566869	-5.37086811282439	-0.12992801373668		
C		0.16601062534209	-4.62707972028064	0.90385496264545		
C		-0.49745512535333	-4.53425687702655	2.29342723602143		
C		5.79850244673851	-1.60215712796259	-0.48324907677038		
C		5.71266823266714	-2.54307462732858	-1.69411508973979		
C		4.30845076596535	-3.14703563057217	-1.78011083829982		
C		3.92603109426064	-3.78760631729852	-0.43768798510906		
C		4.13694216963626	-2.79248935843156	0.71710025757917		
C		3.93181075008259	-3.44351278715649	2.08399169158007		
C		4.92327479894870	3.58981208198030	-0.17787440154783		
C		5.79661556888047	3.07070868650030	-1.32891876751783		
C		5.40722300542757	1.62757104607421	-1.65494702144135		
C		5.45215075552886	0.78225432003396	-0.37271638067783		
C		4.59890967895549	1.42312499477170	0.73118423335966		
C		4.69134803424533	0.67939336205358	2.08127749675663		
C		0.22316788609096	6.00021903891475	-0.25480398240145		
C		1.25885704485041	6.49148156846526	-1.27814210876126		
C		2.26671815299450	5.37964784350193	-1.57451927151976		
C		2.83254764940396	4.80703689437669	-0.26506794305570		
C		1.69570116566228	4.41597121669638	0.69088729335941		
C		2.18002206178925	3.91043008222335	2.06684533492482		

C	-4.59560210890121	3.89436943732031	-0.57869027090341
C	-4.17060748723040	4.78599605388033	-1.76315389076051
C	-2.64727963409602	4.78185972351589	-1.94578880120193
C	-1.96194260255513	5.04283292406540	-0.59722284728272
C	-2.45138886906078	3.99014397198715	0.40945620810525
C	-1.80520397003003	4.05732315314396	1.80398898866000
O	-6.73223992918773	-1.26936230880470	-2.70084181248076
O	-6.08201701219636	1.49318682561241	-3.03294252676664
O	-4.47499832431952	2.55051107677335	-0.94957303830088
O	-6.32933066687720	-0.17320481203527	0.71721711181456
O	-4.69907878976626	0.86185497631448	2.89441765954357
O	-3.59945429078710	-5.93303548930668	-2.13583129184325
O	-5.59074238267987	-3.90137457328215	-2.31406640326279
O	-5.09186157984024	-1.69340666694440	-0.50888978851004
O	-3.55489669760414	-4.55474761918743	1.20622894835606
O	-3.28774338103230	-2.61058073417743	3.27485348506815
O	2.22972084246189	-6.15635022017982	-2.35243000196923
O	-0.63376286367796	-6.26760219676538	-2.39282049083880
O	-1.90425416742196	-4.69428478514283	-0.41829714902407
O	1.40383490146289	-5.31948126561608	1.07398273045718
O	-1.21749287309641	-5.69005304914220	2.64524210876240
O	6.04049963225663	-1.80177404245290	-2.83742699051236
O	4.31914207051608	-4.09160540612562	-2.81806381564641
O	2.56445959458864	-4.16451500046912	-0.56254198110336
O	5.46647455045680	-2.27526764219789	0.70164323585989
O	3.75032090751367	-2.43612511062109	3.05853914585422
O	5.61301982508147	3.93187209052954	-2.41905652296762
O	6.31306331370957	1.15464236358905	-2.61829427111804
O	4.95760833906844	-0.50659415809276	-0.70413581288914
O	5.01978131534536	2.76869163009120	0.95664923133511
O	5.96215784013411	0.15630009954538	2.36029751180396
O	0.55986614037114	6.89069331902484	-2.42453023555716
O	3.28413792109801	5.92727203764689	-2.37300373592739
O	3.60622573429177	3.67441377325382	-0.63505457496323
O	0.84635295697264	5.53821630441627	0.91613368363188
O	3.33478650539735	4.53727683321247	2.55171497919976
O	-4.84122287153134	4.32169062246401	-2.90278557781490
O	-2.33515398094570	5.77632731803488	-2.88831439278250
O	-0.56444167843826	5.00907225052959	-0.84737413721043
O	-3.85500643610568	4.17630735939596	0.57524515057301
O	-1.70552663894151	5.34875653999163	2.34059681095769
H	-7.11765160368575	-1.80819485770410	-0.11041904425354
H	-7.68849611655199	0.12340657311071	-1.51685652372211
H	-4.69009935865141	0.30276152205971	-2.08006839339058
H	-6.48960442375502	2.24659630705728	-0.55441226740647
H	-4.34563421338003	0.33986255621446	0.50664788000551
H	-4.84713854409472	2.58386912326186	1.76486600710725
H	-6.40539644729165	1.79110539280538	2.16287790155100
H	-2.92062965057210	-6.27662460975086	0.42488834234159
H	-5.03328051458779	-5.78225251559121	-0.65673909779820
H	-3.67244832135241	-3.30627062554697	-1.82084953667491
H	-5.89391921548150	-3.44896135717150	0.26326913649275
H	-2.95795236296987	-2.66244707509337	0.61419364714918
H	-4.71984743000635	-1.60035210999977	2.16664714195112
H	3.05211028539792	-6.01766298942222	0.20229001261291
H	1.23222027776360	-7.19520160819024	-0.87204906894862
H	0.24041046535212	-4.47724400251060	-1.85064441590676
H	-0.89570696916201	-6.37812522470946	0.25772479067489
H	0.37156218756954	-3.61133941823902	0.53730718563181
H	-1.14145623411925	-3.65436970989721	2.32246484000752
H	0.30904420920823	-4.41550268001340	3.02399319187103
H	6.83914845651323	-1.27875756360850	-0.35243818402297
H	6.43188444826352	-3.36199124880552	-1.54442461249827
H	3.58666832946662	-2.34342443739050	-1.99463148949151
H	4.55677713386159	-4.67203489705976	-0.27608582113595
H	3.42762809295911	-1.96564025911633	0.58779344333013
H	3.04845449501994	-4.09189063634783	2.04337913749038
H	4.82197663120837	-4.04181759613202	2.30134262967244
H	5.29267667949720	4.57417454285269	0.13865084542905
H	6.84566757051515	3.07905429306428	-0.99804945205595
H	4.37949109499476	1.61160472055944	-2.04712589738240
H	6.49107649026966	0.72465204141660	-0.02321172154994
H	3.55197633365914	1.42915580213520	0.39558667100078
H	4.47111580483720	1.40823045370504	2.86679700207026
H	3.93699003889296	-0.10988163066251	2.10591167377579
H	-0.39485139038612	6.85256401362176	0.05752179628898
H	1.80184049543940	7.33744669448422	-0.83241221353579
H	1.75129343867032	4.56760296962308	-2.10730932720142
H	3.45965265386073	5.56791261719744	0.21744891083901

H	1.10296499031339	3.62216955753762	0.21486757824985
H	1.38576962815226	4.13034651732085	2.78532938684413
H	2.32054051006945	2.82591485092264	2.00944820649994
H	-5.63570794453448	4.12793742842543	-0.31509946026863
H	-4.47057072655434	5.81831080183563	-1.52869329130457
H	-2.32354271788659	3.79337861549088	-2.30945377129727
H	-2.25754115867749	6.03399153066886	-0.22699124342840
H	-2.26733107217932	2.98591090331503	0.00260386464879
H	-0.82583515715703	3.57504888791363	1.74839166929091
H	-2.44518946287523	3.48263389845898	2.47855414295397
H	-5.09708440302018	-3.25629506993396	2.71630930148790
H	-6.88439359894356	-0.78049281034337	-3.52480221849558
H	-5.61340549816846	2.34559683425900	-3.05269133466156
H	-5.00090916130311	1.14427273058527	3.76848474110908
H	-4.25569056826654	-5.90646484779627	-2.85034903948422
H	-5.93840729972902	-3.00809718343168	-2.49383379638013
H	-2.71191333427945	-1.84122548678786	3.15533080472952
H	1.71933761320460	-6.54954649765717	-3.07908045013293
H	-1.58717206157528	-6.07381476402074	-2.33147998119150
H	-2.16405911753326	-5.48640047333130	2.61553822265179
H	5.87510232047575	-2.35947545845281	-3.61499682604115
H	3.55327679780543	-4.68849708925408	-2.72824546920536
H	3.89909524940671	-2.82824654473788	3.93007012075913
H	6.07906673525945	3.55212993392872	-3.18162348017333
H	6.15902721188786	0.20521834867559	-2.77802755767939
H	6.00279919623860	-0.75953749997612	2.03964578486216
H	1.20494244672631	7.19779957175535	-3.08147588946849
H	3.991837511790942	5.27016784486571	-2.49632984760894
H	4.11809731087280	4.07353644056526	2.21171045484131
H	-4.56334279509282	4.86369856967644	-3.65880200463623
H	-1.39882822661490	6.02524792898012	-2.80264601066627
H	-0.84456312809252	5.72564302392559	2.10175405434982
H	0.37359492810761	3.45803289124793	-3.88869152564700
H	0.45892412760692	-0.69058855832264	-4.89386600217130
H	0.47961452524949	-0.11163781844620	-7.28460068252148
H	0.44546762279468	2.25467559689695	-7.95845651648912
H	0.39914261511418	4.03834573098080	-6.28203293429245
H	-4.12555431980972	0.04546191418176	-5.05478348199813
H	-4.11903763374906	-2.42446149500043	-5.14810118008658
H	-2.43943195933334	-3.69657584621441	-3.85975027957255
H	-2.42694811762067	1.23233770704852	-3.72508955942992
H	-0.80471496640330	-2.50435142918757	-2.45704343817281
H	-2.46648626051039	0.44326770658031	-0.53870704796424
H	-2.48373917431082	0.05659389550093	1.90618739556270
H	1.57525798841374	-1.27795056252305	1.69407109100550
H	1.59432978972822	-0.85109002718408	-0.70637403473782
H	1.06351071953764	-2.07304932405723	3.58030247153160
H	0.18364593415641	-1.53902265606994	5.02513819439312
H	2.55780709507385	-0.46279085700888	4.20094539733320
H	1.44004487439233	0.63331234727114	3.37344285262259
H	-0.68174574367192	0.52434961415479	5.47614016090021
H	0.02062619656874	1.55909391182876	6.72381074861927
H	-0.18162354420345	2.21679931659981	3.73992389544019
H	-1.13830437957876	2.92207714369723	5.03769517052569
H	0.58849437544445	3.25668035568069	4.94750492057525
H	2.76298238734736	2.15400156055328	4.96725123410015
H	2.20156610182580	2.12147680827228	6.64950933510591
H	4.48065505458936	1.38643150525398	6.65213436589608
H	3.47720282303108	-0.03258035392541	6.97942430287436
H	4.20698156179363	0.19947070401974	5.38476732561036

E-CL-AV (Fig. S6a)
204

	energy:	gnorm:	xtb:
C	-349.703953988184	0.000385089918	6.4.1 (afa7bdf)
C	-105.28669301800032	42.46038689482494	40.98557037195708
C	-105.63337996125115	41.73557546267617	42.11334751602271
C	-104.67959963316713	40.96999744439375	42.77615581975161
C	-103.38492446358106	40.90668653177885	42.26749403038788
C	-103.04733823623188	41.61507718917873	41.12827991103924
C	-103.99344675960350	42.40207097885963	40.49287816933588
H	-106.01946148557766	43.08005177956940	40.48930182979510
H	-106.64234665400463	41.77180832469452	42.50004479868010
H	-102.65188819089396	40.29132648161561	42.77223988765353
H	-102.04215214380112	41.56497490562609	40.73477294645998
H	-103.72307110471215	42.97157529926308	39.61752870170830
C	-105.02641990908715	40.24964336421846	44.01748863807960
C	-104.37417647472674	40.47908101326593	45.16677177405825
C	-104.51969828956588	39.72735135452585	46.41487073769171
C	-104.62711390047659	40.38028154506735	47.63980926144188

C	-104.51241231717644	38.33267954532549	46.38923538621662
C	-104.75519294754532	39.65674778579157	48.81061316206718
H	-104.62266470267434	41.45977921539339	47.66784375599262
C	-104.63395911125734	37.61355887327888	47.56242602992810
H	-104.40327140759885	37.82408963480057	45.44378537575608
C	-104.76155873388615	38.27257690783438	48.77519124359040
H	-104.850106668678535	40.17892794996822	49.74949875914219
H	-104.62306731499902	36.53524066193320	47.53072709338515
H	-104.85750149622132	37.70927901429842	49.69016313144964
C1	-103.19929166052407	41.78412540319427	45.25905620899054
C	-106.13011290187437	39.27805938331007	43.95410233347504
C	-106.19043437067309	38.36353825454027	42.90893426350737
C	-107.12611654206931	39.24061291277028	44.93160611184457
C	-107.17432508311923	37.39298674512652	42.86276550913407
H	-105.43533742121656	38.39662037518665	42.13636209158368
C	-108.13005130931772	38.30168729773072	44.87057913739216
H	-107.10630288212991	39.95880583451536	45.73658505530184
C	-108.15740962432071	37.35177130182903	43.84551678262898
H	-107.16354157740487	36.67071826995404	42.06441599690309
H	-108.91053289631093	38.26644865086210	45.61222670062962
O	-109.18825938944865	36.46663791559567	43.89264928653049
C	-109.23268358332663	35.37872921036953	42.98413876218660
H	-109.06635512054211	35.71789972634015	41.95705506621633
H	-110.25485797226210	35.00256694060077	43.06900897931345
C	-108.23474254719696	34.26368154032749	43.37500747619031
H	-107.21692306216795	34.65279852929508	43.31464316030957
H	-108.42628076972768	33.99746823818223	44.41927129238321
C	-107.73163859426099	33.17960221872822	41.24790804334909
H	-108.01830229013260	34.12066282710333	40.75391744348929
H	-108.12951656950781	32.36286419072870	40.64433281942603
C	-106.20998877155033	33.05428776654925	41.29593350192526
H	-105.75012369067652	33.93286961097310	41.73864223400079
H	-105.81250098770435	32.92560501891206	40.29332992588629
H	-105.94112446141919	32.18633350645236	41.89086755072697
C	-109.58758905196069	32.37855295448630	42.62649851402015
H	-110.05525272066345	32.61015368605920	43.58556278865635
H	-110.26609827060618	32.72059347078621	41.82752684007827
C	-109.40936034792011	30.86438618429194	42.53364766622447
H	-108.73716403811703	30.52703033504520	43.31679297358187
H	-108.99183063280756	30.57368158292509	41.57389563328489
H	-110.37044180178081	30.37207628224631	42.65436632224547
N	-108.30435338459588	33.05962285493968	42.58171178623319
C	-104.33880399554390	37.73750460797736	38.45961209232616
C	-105.52557101795190	36.75548892883157	38.44341316457317
C	-106.65213090504298	37.37449413624958	39.26965414975808
C	-107.01122702548142	38.76566939660968	38.73001979564987
C	-105.75334344511842	39.63537894787807	38.55758232910664
C	-106.06595954427802	40.88275090394979	37.72101814174598
C	-100.56801894616636	37.20305233747255	42.11739692368077
C	-101.67068976198574	36.13033339339970	42.13475097231286
C	-102.98063172259050	36.73129478155505	41.60456210465083
C	-102.72693353580566	37.30607524032960	40.20946811966966
C	-101.55865877192029	38.30518432071067	40.25937803235144
C	-101.17950302497894	38.79913380557964	38.85662889885943
C	-99.02589954609716	40.24166002409106	46.17207912897711
C	-99.13736243908744	38.71498625657421	46.32257982479771
C	-100.17437102097510	38.15438327823146	45.34080087634759
C	-99.85591384005630	38.64761157886505	43.91686627061468
C	-99.74943276456631	40.18252278885956	43.91991969357930
C	-99.34456704669280	40.73141482434770	42.54733860430687
C	-101.71193598310239	44.12788759494554	48.45430311480617
C	-101.49039530384182	42.92830163395389	49.38734149223170
C	-101.26291134486922	41.67797996681231	48.53716939482409
C	-100.14506703679237	41.91782356271991	47.51488963654485
C	-100.31268772982162	43.24466186489066	46.75441308170603
C	-99.04805292786263	43.62171209854559	45.97836361422675
C	-106.23024876869114	45.72116796138849	46.18878408036468
C	-106.27821265376443	45.40558217839353	47.69764266750221
C	-105.17169875011943	44.40175982817898	48.02545254886135
C	-103.81569403850503	44.94986791026398	47.55857156265679
C	-103.87885512441653	45.40144548437682	46.08964340090225
C	-102.62271153354533	46.19293930663033	45.70376455362263
C	-109.80079222832730	42.95082000765297	43.50491037667762
C	-109.57979904803778	42.56680147302193	44.97698408197640
C	-108.10693036489391	42.81994219142790	45.34353997195389
C	-107.81342021298441	44.29986580906200	45.08272633728006
C	-108.10608554375614	44.62078680548654	43.60470589458304
C	-107.93310860723074	46.11502052284096	43.30160119166638
C	-109.15862187657150	39.72643610527453	39.36053216336839

C	-110.08885083931087	39.26101751810007	40.49249604783744
C	-109.67179469630835	39.96456897188592	41.78729708515567
C	-109.68099060125843	41.48737039494459	41.57385206023690
C	-108.90074446747738	41.87478457574671	40.30646225777858
C	-109.11798472141614	43.35202218657693	39.95627617238524
O	-105.10143282680704	35.52912436016822	38.98500618508601
O	-107.75540723247444	36.49828390469835	39.26193461557096
O	-107.85135967285512	39.37496943700886	39.70257448188539
O	-104.70904360152575	38.94632802561875	37.87378843482696
O	-106.48872992608545	40.55513207285238	36.42428396189424
O	-101.80884510191839	35.65219160373950	43.44502019240516
O	-103.98688327914394	35.74866849393074	41.60928222548372
O	-103.91431192968649	37.95606723040084	39.78578945855833
O	-100.39257610199220	37.70612776065621	40.82216508760961
O	-100.89007500129451	37.74378377312287	37.97795871474926
O	-99.47962115993816	38.43887516188998	47.65348281078290
O	-100.10475941370278	36.75545837931444	45.44840347327157
O	-100.88264285566278	38.22450308570505	43.02975449428461
O	-98.74952051022287	40.59298473594091	44.84527501024246
O	-99.47671129001158	42.12479193875355	42.44506238582546
O	-102.61803642397105	42.80779070379653	50.21278266574353
O	-100.93607961825627	40.61777540069276	49.40176611270697
O	-100.21816572587068	40.80965883044941	46.63084446452221
O	-100.59830575779894	44.33008230382295	47.63171979662177
O	-97.92838714713801	43.52139857131581	46.82812309470234
O	-107.54449504539400	44.90437338322226	48.04591403923977
O	-105.18775359801504	44.17734819973005	49.41258402153241
O	-102.87982698684607	43.89456724296537	47.71993080938265
O	-104.99116265696725	46.26526859587265	45.85762747634749
O	-102.44688615574260	46.30153911796677	44.31802943019062
O	-109.94129787056808	41.22227418690530	45.14555047835501
O	-107.85355739526179	42.42490501239808	46.66563302533498
O	-106.45758110048054	44.57238397772961	45.40086443391161
O	-109.45634050250052	44.29040409882313	43.28058144056524
O	-108.70497177875257	46.92734658242870	44.14681987272222
O	-109.99727997951452	37.86525799607367	40.60840868652053
O	-110.57350932588987	39.57287985029185	42.79187541378254
O	-109.05364035765487	42.08327356079594	42.70102045400077
O	-109.30056264111580	41.10853046835549	39.17372282682283
O	-108.19833891951508	43.82483500703042	39.00850442455384
H	-103.51839466795400	37.34750779186962	37.84447647715455
H	-105.85856824907128	36.62155268466048	37.40527031968455
H	-106.28318166059103	37.51462558992180	40.29349445763534
H	-107.52964325612733	38.67288687414726	37.76699167665487
H	-105.40883021705295	39.93508360630990	39.55546911609321
H	-105.17738365002839	41.52227600077936	37.69567810797212
H	-106.88603057440039	41.42634766758897	38.19098347762839
H	-99.60714146142074	36.73936044657487	42.37355438336601
H	-101.35741053034971	35.31629904596971	41.46313494499623
H	-103.28058508481762	37.54632791277844	42.27931276494580
H	-102.47683222656012	36.48729916903307	39.52269245888540
H	-101.87488984974165	39.15689430088234	40.87165266131300
H	-100.32643855890035	39.48100408653568	38.94449225129868
H	-98.17125724360595	40.61153490013049	46.75255029761847
H	-98.16112494516796	38.27242729525965	46.07354731475240
H	-101.17295149690143	38.52212045738759	45.62134404003064
H	-98.88948963442724	38.23101876398017	43.60519139300796
H	-100.71861750000481	40.60323979945773	44.22609455673983
H	-98.28444311199981	40.52525421986937	42.38976559806932
H	-99.93532914615918	40.22022146656931	41.77858476263368
H	-101.79808718371052	45.04828402266062	49.04698070323832
H	-100.58611337791301	43.11836828725767	49.98277810309661
H	-102.18575156895224	41.44723160554571	47.98527177000186
H	-99.18046647663587	41.93435890172319	48.03847023879371
H	-101.14283910470360	43.13328729501382	46.04505188691676
H	-99.17867013546976	44.64886717255339	45.61983084152612
H	-98.94306274724960	42.94609617635441	45.12094430469849
H	-106.96696807847120	46.50103960981711	45.95280183683044
H	-106.07797801269140	46.34316673844722	48.23529975759777
H	-105.37341940464898	43.46958180168823	47.47590433236105
H	-103.54097615881261	45.80425867278005	48.19192865738241
H	-103.97147366068765	44.51183192654063	45.45314777019905
H	-101.73985663569984	45.67648281067041	46.08526734245265
H	-102.69042077930310	47.18366445208706	46.16997733172089
H	-110.86928847053929	42.88882526007355	43.26125103676551
H	-110.21865526119096	43.21202926756123	45.60057727447927
H	-107.47091107618809	42.20037992895197	44.70011569451207
H	-108.47147081568238	44.90956747071471	45.71446807012312
H	-107.41498276530970	44.04353763937815	42.97750425605195

H	-108.18531768079612	46.28982000810954	42.24998259181270
H	-106.89015629327652	46.38650308640582	43.47050227533411
H	-109.46306666064200	39.27534862437781	38.40761332752798
H	-111.11763092738130	39.55768542723207	40.24162304568083
H	-108.64709459081726	39.65880964095238	42.04350672484114
H	-110.72170280367828	41.82624985397193	41.48883169179956
H	-107.83787332895994	41.68876634155611	40.50096260611274
H	-110.14779633479509	43.47794507424383	39.60348894514907
H	-108.97017456358486	43.95142043308353	40.85661286248110
H	-102.02958925642879	39.33795566302394	38.43284716042988
H	-105.88650235583192	34.96408538519962	39.06852106211328
H	-108.51334884017940	36.94789679974089	39.67806162001562
H	-105.75986754604132	40.10520654582093	35.97239343955366
H	-102.57868050323894	35.06111600214452	43.46672205630588
H	-104.33410743548775	35.63542944464296	40.70190268954227
H	-100.07983788495764	37.30637612646592	38.27824679012951
H	-99.63780601092733	37.48317789532616	47.72391841572983
H	-100.74704420466490	36.34200119958945	44.84081193284039
H	-100.40310108518469	42.37632939577139	42.56320960130795
H	-102.49694471441754	42.01520782292608	50.75925662928626
H	-100.55656172147681	39.88819638369229	48.88283952138629
H	-97.15997622507582	43.89530000515241	46.37392015869953
H	-107.52706902096932	44.71532061622698	48.99941800565917
H	-104.39561408877762	43.67340920806691	49.67240097136305
H	-103.19045052622405	46.79844471751979	43.94795647899313
H	-109.58069601269872	40.93100147778831	45.99878838002398
H	-107.91222797819533	43.20668931942620	47.24883047772649
H	-109.64114848750302	46.77175297905681	43.95303571751563
H	-110.49766496361840	37.61578343953941	41.40160578655747
H	-110.35849942772624	40.04054697538331	43.61939268660952
H	-108.39330775929764	43.41808350767228	38.15231216677935

Z-CL-AV (Fig. S6b)
204

	energy:	-349.704923481810	gnorm:	0.000358911103	xtb:	6.4.1 (afa7bdf)
C		70.70088442980894	-36.03046334027340	-73.79403953256198		
C		70.50290737594983	-35.92748111854957	-75.15908827118767		
C		69.22084133428379	-35.73035476183173	-75.66469350049601		
C		68.14218733842480	-35.67145031157853	-74.78582798009542		
C		68.34312994765682	-35.79965432366158	-73.42401644093948		
C		69.62387644861047	-35.97088792960958	-72.92494944524299		
H		71.69715600389786	-36.16527567235155	-73.40197388561648		
H		71.33999693922524	-35.98317287384779	-75.84260111903208		
H		67.14673637251593	-35.53751406990232	-75.18266218665300		
H		67.49940822408232	-35.77018426438929	-72.75274802067908		
H		69.78651030867778	-36.06458964622816	-71.86312004890331		
C		69.01044326258680	-35.64893024031683	-77.12334786253436		
C		68.26178874301043	-34.67557829265387	-77.66310404746893		
C		67.72478082373618	-33.50758993540210	-76.96294249120670		
C		68.53529725903374	-32.77660899797370	-76.09468370325300		
C		66.41162385335869	-33.09145066213417	-77.17406702226258		
C		68.03469440582421	-31.66497925239617	-75.44421455392884		
H		69.56086959122634	-33.07783802485150	-75.94771054222744		
C		65.91407816201162	-31.98196254590083	-76.51695504969790		
H		65.78222676255758	-33.65043365753749	-77.85197434414101		
C		66.72345628805162	-31.26650405295287	-75.64968490731850		
H		68.67353039179049	-31.10430769344833	-74.77981712501976		
H		64.89391359525135	-31.67360085173108	-76.68596333377808		
H		66.33537807917679	-30.39786305608064	-75.14103148347712		
Cl		67.83383324502287	-34.73994713952229	-79.36938448488735		
C		69.57212808244240	-36.75645037669709	-77.91054747115226		
C		70.28629668190580	-36.54342308242860	-79.08948396787902		
C		69.36726834789528	-38.06461085052143	-77.48639224866493		
C		70.75035746733350	-37.60498695182783	-79.83469049831332		
H		70.49306586923525	-35.53201808062510	-79.41073194964308		
C		69.79369555607720	-39.13842263754850	-78.24612894764370		
H		68.84501216858654	-38.24318611723714	-76.55632423244657		
C		70.48529601927150	-38.91743260233035	-79.43353891975569		
H		71.31557762659698	-37.44843948394796	-80.74098797730265		
H		69.56470667605920	-40.14134783526927	-77.92468977253969		
O		70.94681149743511	-39.90006032178107	-80.24863352046513		
C		70.67336251247869	-41.24975231772004	-79.89969877631597		
H		71.10719800643024	-41.46791208253856	-78.91671674742408		
H		69.59187383376771	-41.42450371539867	-79.86179171496605		
C		71.30094657142556	-42.12192665121688	-80.98493876778784		
H		72.39920110146922	-42.10439225223094	-80.87164942133386		
H		71.06725465960851	-41.65409984940666	-81.94601049550704		
C		70.81301512209201	-44.16101266148539	-79.72691607987380		
H		70.18799749845257	-43.59706234354663	-79.03077375597516		

H	70.33602463379587	-45.13071510352491	-79.87002099552105
C	72.20412461355282	-44.37039049863686	-79.11668377510969
H	72.83771166089406	-44.94787858900816	-79.78530759421022
H	72.69032182767273	-43.42022805675401	-78.91056346625631
H	72.11114716293800	-44.91240056711001	-78.17999540886379
C	71.31698397895654	-44.21947494936740	-82.12537198721715
H	72.39657582046780	-44.41150615881205	-81.99870359537313
H	71.20393408079273	-43.58353485195918	-83.00766439974197
C	70.58716414155177	-45.53316367786318	-82.38256041467422
H	69.51443126037043	-45.36580591729219	-82.36392083504641
H	70.86760869053030	-45.91269226125861	-83.36133299631312
H	70.84167588848797	-46.28651028718346	-81.64256105693593
N	70.75980424171924	-43.46936743882168	-81.00688745015550
C	73.68406538985596	-39.68002847441931	-75.04422123992801
C	74.59136355290858	-38.60157806729218	-74.43072804180912
C	74.27376838985218	-37.25651425516227	-75.08832668768287
C	74.36394694135001	-37.37537208184912	-76.61908678661628
C	73.56474555523897	-38.57903366337892	-77.14246705794598
C	73.90755144836314	-38.85488593563382	-78.61321018294710
C	68.79526076177766	-41.04743801288662	-73.69333040930542
C	69.55938085300210	-40.37912610713929	-72.53902556555109
C	70.68141130565552	-39.51337844026001	-73.11711549907639
C	71.54611958927528	-40.32035059714293	-74.09348988512903
C	70.68671319049005	-41.08304740844426	-75.11333642143086
C	71.51188026233878	-42.09370140050198	-75.92085394992885
C	64.63799034728228	-39.32849297030107	-76.47532835352172
C	64.68275937050622	-38.90971760318657	-74.99640597721844
C	66.13240728712671	-38.87480187160689	-74.50276498412606
C	66.82313133420379	-40.20996231498192	-74.82718858977526
C	66.67003747054147	-40.51890159068807	-76.32692210424088
C	67.26186540613602	-41.86662359073288	-76.75564213818761
C	63.97408979809233	-36.50025734422147	-80.83096784877949
C	62.95684798732773	-36.51353654506471	-79.67433752497494
C	63.67369691081871	-36.78005576857916	-78.34657149535495
C	64.52458336338137	-38.05454275043309	-78.48857757885327
C	65.5097453661741879	-37.85424633329855	-79.64924413973354
C	66.45378574133501	-39.04261365170353	-79.86684763146225
C	66.94765573034533	-32.71222385575469	-82.87355906274571
C	65.65708649602651	-32.13292424388299	-82.27123843637060
C	65.11638357972937	-33.12271108980909	-81.23960803689994
C	64.99099598410717	-34.53520105157175	-81.83083262252418
C	66.24718533774799	-34.95929272167373	-82.61304885436633
C	65.99433665104489	-36.20358666817792	-83.47649150615651
C	71.90554376180062	-32.28368685792206	-81.01292885002346
C	70.97246860970195	-31.08981855586529	-80.74072425835435
C	69.50659302482363	-31.53283725322578	-80.75109478571864
C	69.19971204422927	-32.34151671627574	-82.02189833584869
C	70.22740285054468	-33.47624897892820	-82.18591049329535
C	70.06309346382086	-34.28182835748105	-83.48528361039233
C	74.73430150092209	-35.24914322071513	-77.68770353030038
C	74.34233758228531	-33.84808125366796	-77.18549102120295
C	73.02071333205498	-33.40930711179112	-77.82762683805426
C	73.15203188814743	-33.51636507953515	-79.35252384792020
C	73.57150600425406	-34.94703411616954	-79.73081999226034
C	73.80804547377159	-35.12185287325655	-81.23478981348977
O	74.33954234464294	-38.56886435019195	-73.05003032473373
O	75.18415490030752	-36.31408551386851	-74.57521058904783
O	73.82233597742787	-36.19417752298461	-77.20033397714103
O	73.88188387366944	-39.77013214976906	-76.42798928919389
O	75.27205843365969	-39.11846495372981	-78.79529904053874
O	68.63909935761315	-39.62315374931052	-71.79884119866625
O	71.44945602824851	-39.02012329502539	-72.04734187397079
O	72.35952155540244	-39.35222847978626	-74.73673413464513
O	69.66005582852677	-41.83257358192426	-74.46510958057144
O	72.16470809178830	-43.02402187903003	-75.09931727230438
O	64.04558416445008	-37.66712809908427	-74.87943128300108
O	66.10842010586710	-38.62477877397659	-73.12018126046949
O	68.18159722830224	-40.04740277362431	-74.45381275371597
O	65.28811400659148	-40.55062758393179	-76.66936665040267
O	67.65246745038664	-41.87041926806626	-78.10504762578380
O	62.29910702985131	-35.27556121195109	-79.67788421791219
O	62.68404223718579	-36.89756409662517	-77.35565346152839
O	65.19573750198580	-38.31052790519523	-77.26588700339083
O	64.75588381759336	-37.66294515967254	-80.84742355718967
O	65.80724817700654	-40.28494805047906	-79.89863933673186
O	65.96695568815207	-30.89380816093871	-81.69393979564468
O	63.86658263445111	-32.65601836016725	-80.79902211368002
O	64.76094068771314	-35.35270016140702	-80.69484209022151
O	66.67937429433634	-33.93304374836056	-83.50546197212307

O	67.14857878033683	-36.63448952445953	-84.14603277248635
O	71.34199371043717	-30.52823772238364	-79.51084049724336
O	68.72474609240220	-30.36771936421890	-80.68183395071608
O	67.88749699968803	-32.85331976202694	-81.84881583753840
O	71.54743443144005	-32.94703958901972	-82.18863419167894
O	70.37262173192094	-33.56283418477427	-84.64770051388790
O	74.26600004136516	-33.88214088802940	-75.78733157961798
O	72.76301044149440	-32.09287647852102	-77.41038528373358
O	71.89916119652216	-33.14402998058436	-79.90493361141655
O	74.80201256367874	-35.27096694307315	-79.08651741664332
O	73.94132763247244	-36.47221713964802	-81.59205903860338
H	73.95264200215838	-40.66696286394274	-74.64690954196671
H	75.64066503760594	-38.85914117325066	-74.63087802766485
H	73.24198230478457	-36.98302715822774	-74.83367333673351
H	75.41499029025745	-37.49709953882080	-76.91177472398842
H	72.49353725023263	-38.35817121735974	-77.04605627417844
H	73.29600756897727	-39.68963599687631	-78.97253951168437
H	73.67198709518378	-37.97011691409217	-79.20533302184239
H	68.05263889754163	-41.74721475965152	-73.28816846924306
H	70.00639658506063	-41.16731526128360	-71.91610477092611
H	70.22996474459455	-38.68076383293295	-73.67890331070434
H	72.16614587985784	-41.03206945796626	-73.53168947308791
H	70.23619854891687	-40.34661043804561	-75.78916295749212
H	70.84403505168214	-42.60088834912384	-76.62843312172109
H	63.59463466379314	-39.51482759298721	-76.75977301664363
H	64.14450083272806	-39.67482262168117	-74.41666125130079
H	66.67286756743579	-38.07184364553442	-75.02785358566020
H	66.355446222703032	-41.01118713163558	-74.23970106845906
H	67.16296683874172	-39.71582206043215	-76.88952664664076
H	66.51318146628569	-42.64423089590032	-76.56162002246349
H	68.16252883018342	-42.07889182892714	-76.17692193301936
H	63.43686108499649	-36.49317087319074	-81.78785661858720
H	62.24345654041359	-37.33277814211569	-79.84802378346883
H	64.34795732190362	-35.94000124345227	-78.12492876320540
H	63.87369829777296	-38.90166289239436	-78.73887348981269
H	66.12138865133242	-36.96375952020352	-79.45649616358521
H	67.01638814878662	-38.86279496262977	-80.79065126154734
H	67.15822011072885	-39.07294699102715	-79.03394733941974
H	67.31409640854343	-32.04457419997414	-83.66359753389249
H	64.91780519533143	-32.01624853385410	-83.07667034991587
H	65.82751340886659	-33.17223782390772	-80.40193456049816
H	64.11899814149650	-34.56068862109360	-82.50017309550782
H	67.05126978829145	-35.17162833038799	-81.89619647055932
H	65.6908926946586	-37.02864040327866	-82.83015084294723
H	65.19244942923599	-35.97714207589448	-84.18947310568522
H	72.91972498678874	-31.90742170448553	-81.19971629088343
H	71.11060304896426	-30.36368693027084	-81.55581590937895
H	69.31678467649998	-32.18087889277970	-79.88142427829816
H	69.24095313117569	-31.66510065587514	-82.88565571959090
H	70.10450330471151	-34.16453299255842	-81.33803580377712
H	70.76881811210266	-35.11472931333791	-83.46384745851270
H	69.04329146019404	-34.68117357497631	-83.51853075958348
H	75.75360899526504	-35.48173012498692	-77.35514398783073
H	75.12486545835819	-33.14462618525224	-77.50921947573774
H	72.21229673581506	-34.08065211750641	-77.49777784045899
H	73.93203499164734	-32.81895724868336	-79.68823828498155
H	72.79453308253487	-35.64724993754448	-79.39784428115698
H	74.70177362707253	-34.55211760577051	-81.51576030522084
H	72.94983230817758	-34.73853944779133	-81.78912420961102
H	72.28940614078363	-41.56198665988488	-76.47313838930431
H	74.87163956518388	-37.85174906179937	-72.66887039858065
H	74.92948779208976	-35.42366931834539	-74.87930255263520
H	75.49642486968081	-39.92080743821376	-78.30121406121961
H	69.12852211661159	-39.15915510072921	-71.10180099282746
H	72.33219015412784	-38.77630088221716	-72.37632957600003
H	71.49253305039593	-43.53030169264660	-74.61926726283382
H	64.11140654692352	-37.38038864025842	-73.95471070885992
H	66.96962884902257	-38.86297679916880	-72.73192616379650
H	66.88659602348778	-41.63278403692328	-78.65493596724774
H	61.71422338907789	-35.25076650821799	-78.90286339121164
H	63.10623884885933	-37.02393863185471	-76.48600391565377
H	65.28051722551463	-40.34774801748595	-80.70855470165830
H	65.17642681684241	-30.57103862106429	-81.23177706334553
H	63.40669634009221	-33.37315303399952	-80.33186254947780
H	67.38116630077292	-35.98115643487827	-84.82100390870507
H	70.72383021869301	-29.80663130941354	-79.31071762440942
H	67.79878071559570	-30.57441711890467	-80.90618470565347
H	69.72945923091802	-32.85542412616469	-84.78889255769967
H	73.93260451112526	-33.02151565651793	-75.48523957411358

H	72.19882734047290	-31.64441389567656	-78.06603280725018
H	74.74141633706247	-36.82505154561426	-81.17612148199287