

Lycopene interactions with β -Cyclodextrins: Raman Spectroscopy and Theoretical Investigation

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SUPPLEMENTARY MATERIAL

List of Material

Figure S1. MD simulations showed that after 1 ns the structure was no longer as complexes what can be clearly seen according RDMS, Mass of centre.

Figure S2. Clustering of water molecules while the number is small in simulation box: Lyc and CD complex with 1000 (A) and 10000 (B) water molecules.

Figure S3. Lycopene with an artificial CD: A and B from different sides.

Table S1. Cartesian coordinates of artificial CD with lycopene

Table S2. Cartesian coordinates of β -Cyclodextrin with lycopene at ending group position (see Figure 7 C)

Table S3. Cartesian coordinates of β -Cyclodextrin with lycopene at central position (see Figure 7 D)

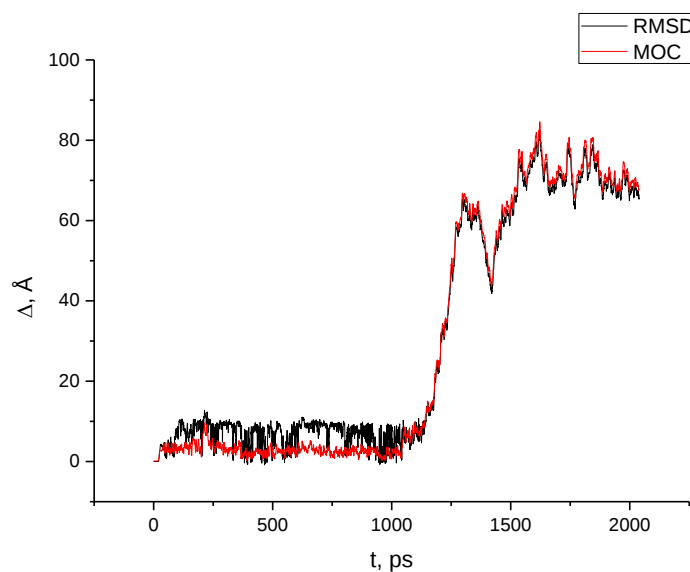
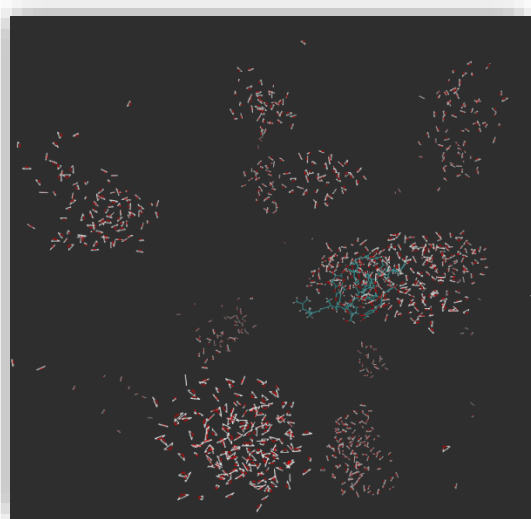
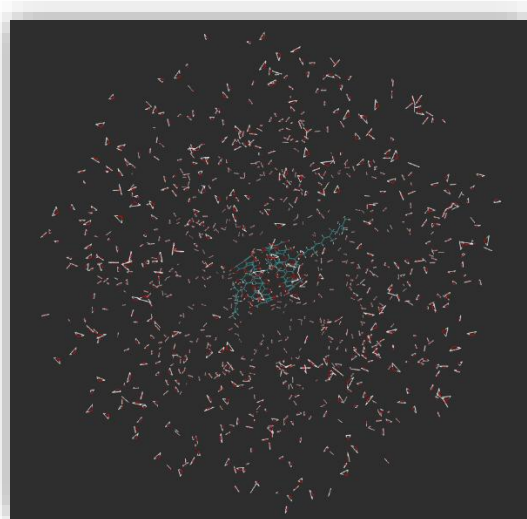


Figure S1. MD simulations showed that after 1 ns the structure was no longer as complexes what can be clearly seen according RDMS, Mass of centre.

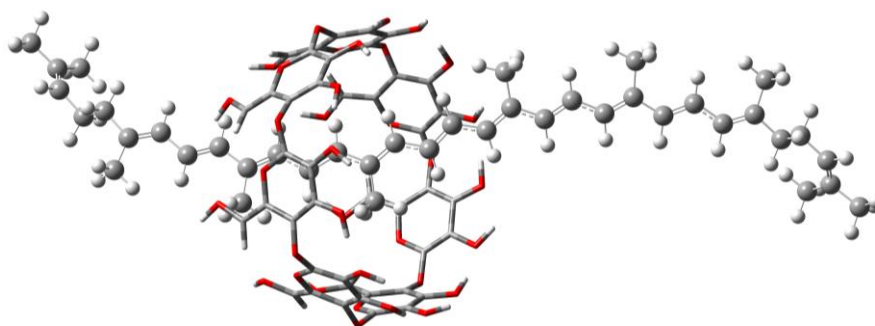


A

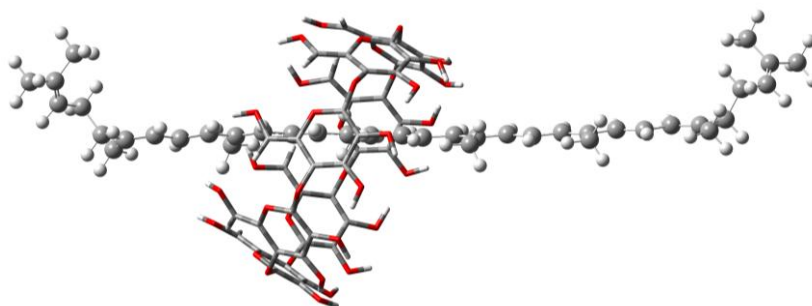


B

Figure S2. Clustering of water molecules while the number is small in simulation box: Lyc and CD complex with 1000 (A) and 10000 (B) water molecules.



A



B

Figure S3. Lycopene with an artificial CD: A and B from different sides. Cartesian coordinates presented in Table S1.

Table S1. Cartesian coordinates of artificial CD with lycopene

C	13.04394900	-4.99121700	-3.22373100
C	11.99798200	-5.38503300	-4.23696200
H	12.46188200	-5.56633400	-5.22346500
H	11.20998900	-4.63181100	-4.36889600
H	11.51466600	-6.33484400	-3.94520800
C	14.12347500	-6.02457800	-3.00900900
H	14.65597900	-6.24406500	-3.95245200
H	13.69238600	-6.98318300	-2.66707900
H	14.86548500	-5.69801300	-2.26524500
C	13.06085600	-3.82777200	-2.54844100
C	12.08096300	-2.68831000	-2.61661100
C	11.36070400	-2.45150900	-1.26313700
C	10.39542900	-1.28744500	-1.26961700
C	11.01574000	0.08315100	-1.35146900
H	11.73962400	0.22768900	-0.52921400
H	10.28087800	0.89707900	-1.29978600
H	11.58522500	0.20958900	-2.28910600
C	9.05765900	-1.51373200	-1.20522200
C	7.98691500	-0.53917900	-1.21126700
C	6.66612300	-0.87548100	-1.13995800
C	5.53283800	0.02980900	-1.13963800
C	5.79208000	1.50978300	-1.25899900
H	6.35313900	1.87143500	-0.38092600
H	4.87332900	2.10547600	-1.31499600
H	6.39954600	1.73240300	-2.15372800
C	4.28304400	-0.51481900	-0.97630600
C	3.02289800	0.16859400	-0.91107200
C	1.86595600	-0.48168900	-0.58059000
C	0.54418900	0.09226700	-0.49318600
C	0.34275500	1.52657700	-0.91062400
H	0.96948900	2.20186300	-0.30388900
H	-0.69777800	1.85700100	-0.80366000
H	0.64046200	1.67810200	-1.96134500
C	-0.47289500	-0.71346700	-0.03150000
C	-1.86597300	-0.41222300	0.07721900
C	-2.78264200	-1.28850300	0.60270400
C	-4.19254000	-1.04677100	0.63257300
C	-5.18450400	-1.84915100	1.15945400
C	-4.89866800	-3.15908100	1.85476300
H	-3.83587100	-3.42543100	1.83369300
H	-5.45627500	-3.98608600	1.38464400
H	-5.21989800	-3.11578400	2.90965500
C	-6.55465600	-1.40484200	1.06020600
C	-7.66051900	-2.05827200	1.53221000
C	-8.99302200	-1.54685200	1.39276300
C	-10.16797900	-2.11428600	1.82308800
C	-10.23025500	-3.43568300	2.54860300
H	-9.24187900	-3.88782900	2.69543800
H	-10.85028800	-4.15932600	1.99262300
H	-10.69527200	-3.31627600	3.54195800
C	-11.40808100	-1.40987700	1.56612100
C	-12.66082700	-1.81708000	1.91376600
C	-13.85277900	-1.05393000	1.61566600
C	-15.14018900	-1.36760700	1.91502200
C	-15.55553700	-2.61511200	2.65092200
H	-14.70675500	-3.20817000	3.01539900
H	-16.16875300	-3.27284800	2.00967700
H	-16.18600600	-2.35717800	3.52077900
C	-16.25997800	-0.44074300	1.49831700
C	-17.17032500	-1.00835100	0.37765500
C	-18.29008600	-0.06864400	0.02235500
C	-18.52362200	0.55468100	-1.14678500
C	-17.67503300	0.40990000	-2.38558800
H	-18.27495600	0.00905800	-3.22266300
H	-16.80703300	-0.24824000	-2.24792100
H	-17.30378900	1.39613600	-2.71783200
C	-19.70844700	1.47654000	-1.30736300
H	-20.37669600	1.12675000	-2.11541600
H	-19.38375100	2.49364100	-1.59346100
H	-20.30034200	1.55310400	-0.38307300
H	-17.60571800	-1.96473000	0.72121000
H	-15.84114200	0.51916500	1.15580900

H	-13.68109400	-0.11009600	1.08361600
H	-9.07549100	-0.58309100	0.87588600
H	-7.52740300	-3.01632100	2.04001900
H	-6.70951000	-0.44405900	0.55446200
H	-4.51985000	-0.10964500	0.16591900
H	-2.40583100	-2.23774300	0.99329100
H	-2.23034000	0.54835100	-0.30155800
H	-0.18907400	-1.72645500	0.27561600
H	1.93596700	-1.55162700	-0.35573200
H	2.99710300	1.24229200	-1.11257700
H	4.23068900	-1.60358600	-0.86423600
H	6.41367000	-1.93989400	-1.06329800
H	8.25562000	0.51756500	-1.28280800
H	8.73484800	-2.56023700	-1.13653000
H	10.82881200	-3.37528300	-0.98392500
H	11.32353800	-2.85011000	-3.39879900
H	-16.54794400	-1.24815600	-0.49797400
H	-18.99107800	0.13478100	0.84318300
H	12.62608600	-1.76824600	-2.89722000
H	12.13085300	-2.28399800	-0.48581000
H	13.88392300	-3.67765900	-1.83680900
H	-16.89399000	-0.21364000	2.37709000
H	-11.31035000	-0.45517000	1.03527100
H	-12.78059100	-2.76685300	2.44066600
C	0.45696300	-4.95192800	0.08224000
C	-0.09131000	-4.92673300	1.31042100
C	0.75967900	-4.68969400	2.46823500
C	2.09263000	-4.52058300	2.27660500
C	2.66284100	-4.49730900	0.93642600
C	3.95359800	-4.26222600	0.62532000
O	1.78067700	-4.72558100	-0.13638300
O	0.09325700	-4.71452200	3.64895700
O	-1.43979200	-5.14474200	1.51080000
O	-2.43698100	-1.64471100	-4.52374700
O	4.35102800	-4.21541500	-0.69637400
H	0.62131400	-4.27552900	4.35552500
H	-1.58924600	-5.09039200	2.47134800
H	4.68653700	-4.03476900	1.39566500
H	5.31734300	-4.21865900	-0.70765500
C	-1.98963600	2.48434900	-4.28851500
C	-3.04748600	1.91745200	-3.68337100
C	-3.20341600	0.46968200	-3.72847200
C	-2.24649400	-0.26954700	-4.34454100
C	-1.05090600	0.35783700	-4.89308600
C	0.03954500	-0.27272100	-5.37261900
O	-1.03981400	1.76569500	-4.94166500
O	-4.34499400	0.02843200	-3.14514500
O	-4.00414500	2.66912400	-3.03052900
O	-1.81433900	3.82911600	-4.40869300
O	1.09900400	0.44950700	-5.87350200
H	-4.30134500	-0.94575700	-2.97866100
H	-4.66701900	2.03917400	-2.69653500
H	0.10542900	-1.35820800	-5.36461800
H	1.81032200	-0.17984600	-6.05147900
C	0.38389200	6.10030600	-1.70440000
C	-0.93596400	5.95090600	-1.49663000
C	-1.71150600	5.12717200	-2.41405200
C	-1.07058600	4.50897500	-3.43868500
C	0.37455600	4.61657900	-3.59443400
C	1.13944500	3.95213900	-4.48516200
O	1.03715000	5.52317900	-2.74656700
O	-3.03836200	5.09781500	-2.13111700
O	-1.58380400	6.56733900	-0.44538800
O	1.18032000	6.92594100	-0.97268300
O	2.49815100	4.16658000	-4.53165400
H	-3.46936800	4.32527600	-2.56267900
H	-2.50878100	6.26500300	-0.47730200
H	0.70031900	3.23646700	-5.17625000
H	2.86043700	3.54784400	-5.17940200
C	3.31309100	5.69653300	2.37704900
C	2.07428000	6.18995300	2.54821800
C	1.29657000	6.58188000	1.38181600
C	1.84260900	6.41672100	0.15036900

C	3.15535400	5.80446000	-0.01617700
C	3.74662500	5.49534200	-1.18834200
O	3.88527800	5.53053800	1.15678400
O	0.08448200	7.10988400	1.68600100
O	1.51963900	6.34120900	3.80415600
O	4.15096900	5.40593300	3.40880900
O	5.00300800	4.93359900	-1.20937300
H	-0.51273600	7.08004100	0.90397700
H	0.60627800	6.64877600	3.66319800
H	3.23992500	5.67430700	-2.13369600
H	5.21660500	4.74201600	-2.13201200
C	4.59653400	1.52882000	4.85368200
C	3.62691200	2.30184100	5.37472500
C	3.41610000	3.64035400	4.84161500
C	4.23023800	4.07883900	3.84887200
C	5.27905500	3.23154200	3.30220800
C	6.14044700	3.57889400	2.32522400
O	5.41073600	1.94396300	3.84720200
O	2.40801500	4.31269700	5.44911000
O	2.82762900	1.87032300	6.41486000
O	4.92743400	0.30003200	5.33099600
O	7.08829200	2.68120500	1.88116600
H	2.16033500	5.12410700	4.94780200
H	2.16033000	2.56530500	6.55542900
H	6.05916200	4.54482800	1.83195900
H	7.70640800	3.16315200	1.31642600
C	3.31711800	-3.24551800	3.86490500
C	2.66355300	-2.60509500	4.84865600
C	3.20121100	-1.35117900	5.36015700
C	4.31860900	-0.83796400	4.78424800
C	4.95508100	-1.50377100	3.65386700
C	5.97683700	-1.03975100	2.90536200
O	4.47783900	-2.79057100	3.33057900
O	2.49252300	-0.84656800	6.40160000
O	1.49605300	-3.10143900	5.39409000
O	2.94916900	-4.46507600	3.38022900
O	6.50861400	-1.81761300	1.90852700
H	2.68935000	0.10995500	6.53035700
H	1.19096900	-2.43630700	6.03658000
H	6.40796300	-0.05793200	3.09408000
H	7.00754800	-1.24439600	1.30559900
O	-0.22002100	-5.29881100	-1.04472300
C	-1.95686800	-2.50088900	-3.58160100
C	-2.69555200	-2.98642300	-2.56740600
O	-0.68767300	-2.90838200	-3.83843700
C	-2.09785600	-3.96630100	-1.66912600
O	-3.99713900	-2.57068000	-2.36589800
C	0.00310800	-3.70843600	-2.91179900
C	-0.79216800	-4.29835600	-1.84416200
O	-2.93862600	-4.44011400	-0.71810700
H	-4.21272600	-2.71371700	-1.42517900
C	1.32310100	-3.88308500	-3.12546900
H	-2.43559900	-4.88678200	-0.00353600
O	1.93907800	-3.28906000	-4.20402500
H	1.91966700	-4.50205000	-2.45889400
H	2.89193800	-3.39075600	-4.07915300

Table S2. Cartesian coordinates of β -Cyclodextrin with lycopene at ending group position (see Figure 7 C)

C	5.96637100	4.78114000	-2.94498900
C	6.88929100	5.04721200	-1.73855600
C	6.02774700	5.34268400	-0.49131500
C	4.64455800	5.87235900	-0.92377200
C	3.91053300	4.75120800	-1.69231700
C	2.69342700	5.18287800	-2.50242700
O	4.84322500	4.03261500	-2.53434400
O	6.74669600	6.25293200	0.30651400
O	7.76194300	3.93630500	-1.50854400
O	6.45824400	-1.01999400	-5.82373600
O	1.91225800	4.05413500	-2.89164200
H	6.20070900	6.43891700	1.09940900
H	8.24924200	4.13333000	-0.69283400
H	2.09085900	5.89280800	-1.90517500
H	1.56303600	3.66465300	-2.06074500
C	4.96541200	-4.24437200	-3.73036100
C	6.50665100	-4.27657700	-3.93930000
C	7.00919000	-2.85523200	-4.19488400
C	5.96158000	-2.12833600	-5.05220700
C	4.74168400	-1.86429200	-4.13606600
C	3.45265700	-1.51476900	-4.89067600
O	4.55559400	-2.98726700	-3.22415600
O	8.28925800	-2.96684000	-4.77872800
O	7.22590100	-4.83750700	-2.84292900
O	4.39976000	-5.31484900	-3.01792300
O	2.60531300	-0.65337400	-4.14826200
H	8.65304500	-2.06138800	-4.73845200
H	8.16194600	-4.65792400	-3.03560500
H	3.71886900	-1.06661700	-5.86278400
H	2.76657900	0.27190600	-4.43263300
C	3.62906700	-5.65652900	1.00976800
C	4.96741500	-6.31810500	0.63291100
C	5.41943300	-5.79855700	-0.74631100
C	4.18227500	-5.45325900	-1.60396900
C	3.40527300	-4.29151400	-0.91920100
C	1.90965000	-4.31520000	-1.25061300
O	3.62716600	-4.33550300	0.51016300
O	6.23108200	-6.80531800	-1.30845500
O	5.95371500	-6.02961600	1.62331100
O	3.37850400	-5.73814100	2.39244100
O	1.15052200	-3.35158000	-0.52856800
H	6.70095200	-6.36437400	-2.04327200
H	6.78844100	-6.40508400	1.30232100
H	1.80061100	-4.18603900	-2.34224000
H	1.42612500	-2.45046100	-0.77805600
C	2.56072100	-2.57798500	4.85599100
C	4.07695800	-2.87199800	4.80744700
C	4.36932600	-3.85255700	3.64983000
C	3.10041300	-4.63796200	3.26652200
C	2.01190400	-3.66185700	2.77525700
C	0.59713000	-4.22791000	2.74163400
O	2.04641300	-2.44024400	3.54622200
O	5.40756000	-4.71605100	4.06337700
O	4.81613700	-1.65657400	4.67936200
O	2.15426100	-1.51613400	5.67877900
O	-0.27857900	-3.37462000	2.01110600
H	5.59252300	-5.31268100	3.30845600
H	5.69448000	-1.84695900	4.30085200
H	0.62251400	-5.24351800	2.30225400
H	0.05055100	-3.35939600	1.08743900
C	1.54779500	2.47793400	4.69689600
C	2.78799100	2.17033200	5.59626900
C	3.25224800	0.73775400	5.35046800
C	1.98864100	-0.13351800	5.33201100
C	1.25137600	0.16711400	4.00350800
C	-0.22970500	-0.23641400	4.02763000
O	1.45910500	1.55563000	3.61880300
O	4.18570700	0.43012800	6.36455300
O	3.88253000	3.06207400	5.41214600
O	1.37695400	3.79202600	4.24647000
O	-0.73050800	-0.61639600	2.75830700
H	4.62129600	-0.38727300	6.05115400

H	4.62319200	2.63283000	5.87646000
H	-0.35570300	-1.05171400	4.76326800
H	-0.51993800	-1.56319600	2.60474200
C	3.21444600	5.81317000	1.16670300
C	3.70376700	6.26246200	2.56142400
C	3.40438800	5.13605000	3.55610600
C	2.05127000	4.48615300	3.18448000
C	2.25903400	3.73269300	1.83939900
C	0.98175400	3.60325900	1.00326600
O	3.29990500	4.40366300	1.08195600
O	3.44955800	5.69395100	4.85064200
O	5.10027200	6.54634000	2.54950200
O	3.89985200	6.47915900	0.13461500
O	1.21992800	3.03317000	-0.28236200
H	3.54983900	4.92165400	5.43848600
H	5.36262800	6.63131400	3.48058900
H	0.24952400	3.01229500	1.57821300
H	1.34518200	2.06970600	-0.18991100
O	6.59236100	4.22834600	-4.07679000
C	6.56468500	0.32166000	-5.43216000
C	7.89288300	0.74228000	-4.74324200
O	5.44968700	0.69787200	-4.65177800
C	7.65164400	1.95627300	-3.83784100
O	8.47971300	-0.32146700	-3.99377800
C	5.25229200	2.11239100	-4.42606500
C	6.60001400	2.86045400	-4.50828200
O	8.90480400	2.56861200	-3.62792000
H	9.22465500	0.08090800	-3.51646100
C	4.13305700	2.64150100	-5.31775200
H	8.74805400	3.22122200	-2.91642800
O	2.86421900	2.16289500	-4.88277900
H	4.15942000	3.74438000	-5.32535400
H	2.54252600	2.76999000	-4.17888900
H	2.99670600	5.69986800	-3.42764900
H	4.27821300	2.29359800	-6.35492700
H	2.89404400	-2.44624100	-5.09393200
H	1.46892800	-5.29121800	-0.99040600
H	0.18248500	-4.31629900	3.75944500
H	-0.83410000	0.61939700	4.37576600
H	0.54072100	4.59599800	0.81700500
H	2.66981700	2.73551300	2.03615000
H	3.57086100	4.01029500	-0.96381300
H	4.89746900	2.16465200	-3.39586200
H	4.97872500	-1.03370600	-3.47030300
H	3.83637000	-3.33451300	-1.22804500
H	2.26480700	-3.35150600	1.75872700
H	1.73800000	-0.39478900	3.20538400
H	1.33243200	5.30860300	3.02423700
H	4.80801700	6.74497500	-1.57790400
H	6.89585900	2.99130700	-5.56400300
H	5.66869900	-2.80913400	-5.87068200
H	3.54649700	-6.3555700	-1.61038100
H	2.75740200	-5.17479100	4.16668700
H	1.35816600	0.19346900	6.17870500
H	3.73541900	0.70127000	4.35844500
H	4.19714100	4.38057600	3.43435300
H	5.86511500	4.38139900	0.03631900
H	7.23545500	1.58554100	-2.88238700
H	7.07643600	-2.34633300	-3.21631600
H	5.99757000	-4.87174100	-0.57908600
H	4.66714800	-3.25521900	2.76634400
H	2.44952800	2.23714400	6.64844200
H	3.14363700	7.16658900	2.86538900
H	7.48567000	5.95234300	-1.95332400
H	8.59457700	1.05630100	-5.53902000
H	6.70383200	-4.87784900	-4.84711400
H	4.82074500	-7.41084400	0.55586300
H	4.35710200	-3.37992600	5.74831800
H	0.66330500	2.34815100	5.34759600
H	2.15528000	6.12136400	1.07113700
H	5.64071800	5.77526800	-3.30665200
H	6.53755300	0.85794300	-6.40020000
H	4.52934200	-4.38731600	-4.73708700
H	2.82211200	-6.23655700	0.52090500

H	2.09429300	-3.45148500	5.35044800
C	-21.29968200	0.54172000	0.22666400
C	-19.97843400	0.52871000	-0.08843200
C	-18.85454800	0.33194800	0.80084400
C	-17.55914900	0.34226200	0.37902600
C	-16.38040100	0.15547300	1.20105500
C	-15.14774200	0.20026500	0.59601900
C	-13.85739900	0.04679800	1.20294400
C	-12.68657300	0.11253200	0.49756900
C	-11.35253500	-0.02785000	1.03011300
C	-10.28753900	0.07132300	0.16188700
C	-8.89357000	-0.02963900	0.46064900
C	-7.90321800	0.08702300	-0.48162800
C	-6.50968700	-0.01006100	-0.17951600
C	-5.44233300	0.09441300	-1.04427100
C	-4.11083600	-0.03356900	-0.50275000
C	-2.93554800	0.04576200	-1.19983600
C	-1.65484800	-0.08815900	-0.56873700
C	-0.41697000	-0.01547500	-1.16523500
C	0.73577700	-0.15890700	-0.29457900
C	2.06418600	-0.09513800	-0.63546900
C	3.10349600	-0.19974700	0.37734300
C	4.43508800	0.04066800	0.25740400
H	-19.71651800	0.68773500	-1.14181800
H	-17.37126400	0.50775600	-0.68879800
H	-15.14006200	0.37608000	-0.48651300
H	-12.75280900	0.29060200	-0.58245600
H	-10.53177600	0.25176200	-0.89196600
H	-8.20584500	0.26592200	-1.51826300
H	2.74355000	-0.46457500	1.37715500
H	0.49087000	-0.31530500	0.76288200
H	-1.67162400	-0.25273000	0.51481400
H	-4.04714100	-0.20966300	0.57741100
H	-6.26721200	-0.18833300	0.87499300
H	-8.58948700	-0.20857800	1.49681900
H	-19.06396800	0.16607700	1.86041900
H	-13.81255200	-0.12977100	2.28010100
H	2.35263300	0.03887000	-1.68254800
H	-2.96829100	0.22221700	-2.27745500
H	-21.83743400	1.06968700	-1.78822000
C	5.31867900	-0.03320000	1.48347600
C	8.03836100	-1.97166800	3.21774400
C	8.10819000	-3.37366100	2.66785100
H	9.15255400	-3.62634700	2.40880500
H	7.48774600	-3.52437000	1.77506500
H	7.77267500	-4.09582200	3.42898700
C	8.83204400	-1.75532500	4.48512300
H	9.90091000	-1.98270600	4.32100300
H	8.49246700	-2.43530500	5.28680900
H	8.75522600	-0.72086500	4.85232900
C	7.36307700	-0.95476900	2.64412100
C	6.55058200	-0.95991200	1.37232000
C	5.09479600	0.46595500	-1.02481900
H	5.58592200	1.44920500	-0.90562400
H	4.38771900	0.54036700	-1.85930200
H	5.88583800	-0.24289400	-1.32444500
C	-0.20671900	0.24765700	-2.63384600
H	0.19225100	1.26659300	-2.78894800
H	-1.13709900	0.17163500	-3.21101100
H	0.52933600	-0.43876100	-3.07951400
C	-5.60084600	0.33765600	-2.52517800
H	-5.09316900	1.26959400	-2.82643900
H	-6.65052100	0.41511800	-2.83348000
H	-5.13974200	-0.47763700	-3.10790300
C	-11.18850300	-0.27467700	2.50997000
H	-10.13827900	-0.36836200	2.81140300
H	-11.70750700	-1.19968800	2.81345800
H	-11.63328100	0.54696800	3.09669300
C	-16.56693600	-0.07748400	2.68007400
H	-15.61727500	-0.20578700	3.21357300
H	-17.17755400	-0.97841600	2.86155100
H	-17.10180800	0.76753900	3.14622700
C	-21.83579600	0.35326200	1.62233900

H	-21.04955300	0.30862700	2.38712400
H	-22.42923200	-0.57491100	1.70244500
H	-22.51881400	1.18016000	1.88791800
C	-22.33325300	0.75088400	-0.85722600
C	-23.19670500	-0.50101600	-1.16318200
C	-24.23444500	-0.23365100	-2.21894600
C	-24.35508000	-0.79006400	-3.43787500
C	-23.43772600	-1.84934600	-3.99656900
H	-24.00434400	-2.76795500	-4.23422700
H	-22.62049000	-2.12408500	-3.31674700
H	-22.98858000	-1.51022900	-4.94745200
C	-25.47120400	-0.37882900	-4.36774900
H	-26.10485300	-1.24441900	-4.63458100
H	-25.06991600	0.01533100	-5.31929700
H	-26.11645900	0.39299600	-3.92224400
H	-23.70839000	-0.81736500	-0.23558300
H	4.71995800	-0.34943500	2.35182300
H	6.22386900	-1.97829900	1.10646100
H	-22.53138900	-1.33032300	-1.44821700
H	-24.97425400	0.53109700	-1.94610600
H	7.19109700	-0.61461800	0.53896700
H	5.68806500	0.98799600	1.70946900
H	7.42798800	0.02491800	3.13747100
H	-23.01172800	1.57480800	-0.56241300

Table S3. Cartesian coordinates of β -Cyclodextrin with lycopene at central position (see Figure 7 D)

C	2.28982800	-0.77963000	5.66612400
C	1.23664700	-0.11572400	6.58713500
C	0.91403800	1.29956600	6.07795100
C	2.16292900	1.88756300	5.39203100
C	2.39740900	1.07118500	4.10049800
C	3.75563100	1.25382300	3.42988100
O	2.13859600	-0.33311900	4.33695300
O	0.46046500	2.04041600	7.18746700
O	0.04078500	-0.89082700	6.67843600
O	0.29202500	-5.96680300	2.29983700
O	3.73308400	0.78031200	2.08402700
H	0.10959700	2.87325600	6.81199500
H	-0.58359200	-0.35572900	7.19510200
H	4.04396700	2.31792200	3.46895800
H	3.36071400	1.49633300	1.52129200
C	-1.91070300	-5.45005300	-1.12122500
C	-2.78136300	-5.91205200	0.07058500
C	-2.03397900	-5.63604300	1.38722800
C	-0.51455300	-5.73810200	1.13409300
C	-0.12031500	-4.54111900	0.23536000
C	1.24376200	-4.64779400	-0.44129200
O	-1.14973000	-4.32144900	-0.76017700
O	-2.52431500	-6.55355900	2.33796000
O	-4.05398900	-5.26598300	0.07605100
O	-2.60106400	-5.24671600	-2.33064400
O	1.64488700	-3.40839000	-1.02054100
H	-2.16824900	-6.24355600	3.19441600
H	-4.48324400	-5.52060400	0.90879700
H	1.98884500	-4.99924500	0.29100900
H	2.06019100	-2.86845600	-0.31971100
C	-3.76748000	-1.73407600	-4.10804600
C	-4.93134000	-2.42620400	-3.35940200
C	-4.37273900	-3.45668900	-2.36059800
C	-3.03595600	-4.00308200	-2.89957100
C	-2.01441500	-2.84212100	-2.86128700
C	-0.74483700	-3.07423200	-3.67493000
O	-2.65157600	-1.60028600	-3.25763600
O	-5.36695400	-4.44012700	-2.18684000
O	-5.76047300	-1.47637100	-2.68696900
O	-4.10036800	-0.52112000	-4.73932300
O	0.28210100	-2.14778700	-3.33036700
H	-5.06067200	-4.97803800	-1.42916800
H	-6.37832100	-1.98698000	-2.13815900
H	-0.40311300	-4.11188500	-3.52500000

H	0.73182900	-2.48459600	-2.52358800
C	-3.21523700	3.35717600	-3.65608700
C	-4.67443700	2.95121800	-3.32240600
C	-4.79269200	1.41971300	-3.29271600
C	-3.80637000	0.81954500	-4.31515000
C	-2.38664800	1.07063100	-3.75650800
C	-1.22712900	0.83857800	-4.72337500
O	-2.30226400	2.39328800	-3.17814400
O	-6.14733800	1.10415000	-3.52416500
O	-5.10854300	3.50245500	-2.08125300
O	-2.83108900	4.64874300	-3.26196300
O	0.00304100	0.66367400	-4.02191600
H	-6.22065700	0.13901600	-3.37896600
H	-5.95599700	3.07585000	-1.87261600
H	-1.44758000	-0.03562500	-5.35942400
H	0.07183400	-0.28471100	-3.77403900
C	-0.80930300	5.89916600	0.08213700
C	-2.32661800	6.18351700	0.17372800
C	-3.07196600	5.28989100	-0.83189800
C	-2.16037800	5.04530200	-2.05334300
C	-0.99130600	4.14962900	-1.57381700
C	0.22273300	4.11267900	-2.49891900
O	-0.58951300	4.54575800	-0.23819500
O	-4.28839000	5.93480600	-1.13382100
O	-2.82710000	5.96624600	1.49329400
O	-0.05239100	6.30520100	1.19616700
O	1.10502300	3.04206200	-2.17437900
H	-4.81319800	5.26203300	-1.61100700
H	-3.79237900	6.05133900	1.43042300
H	-0.11909900	4.04166100	-3.54474200
H	0.76315100	2.23860600	-2.61186400
C	1.54818900	4.08815700	4.24533300
C	0.22903400	4.77662500	4.66482400
C	-0.54895200	5.20869500	3.40688600
C	0.45020400	5.49295000	2.26562500
C	1.08979000	4.14138000	1.86773200
C	2.34867800	4.23929400	1.01112800
O	1.35587600	3.35612200	3.05740900
O	-1.33806400	6.31749100	3.77001000
O	-0.57540500	3.92042800	5.47789100
O	2.16946900	3.31542300	5.24521600
O	2.70698600	2.97678400	0.45624900
H	-1.93338300	6.46770200	3.00781800
H	-1.41123200	4.39274100	5.62180200
H	2.19251700	4.98806300	0.21715800
H	2.17975800	2.84340300	-0.35930500
O	2.36438700	-2.18112900	5.73285000
C	0.78169100	-5.02104100	3.21575500
C	-0.03659200	-4.86025900	4.52081600
O	0.98700200	-3.76565100	2.60950400
C	0.29354200	-3.50679800	5.17158000
O	-1.44124400	-4.96484900	4.28910000
C	1.84028400	-2.85127000	3.34034500
C	1.75920700	-3.14744400	4.85710300
O	0.00615100	-3.63041900	6.54597300
H	-1.86699000	-4.75209800	5.13562700
C	3.24897000	-2.84461800	2.75090400
H	0.05640000	-2.71858200	6.89571300
O	3.28723600	-2.19486500	1.48492200
H	3.93884400	-2.36568600	3.46667200
H	3.38957300	-1.23665400	1.65236200
H	4.52629700	0.67553100	3.96693200
H	3.59378600	-3.88171600	2.59641100
H	1.20009300	-5.38626700	-1.26026200
H	-0.95422000	-2.94231700	-4.75031200
H	-1.10742800	1.71393100	-5.38377400
H	0.79975200	5.04781700	-2.39553000
H	3.19991600	4.57573100	1.62776100
H	0.35173500	3.55076100	1.32126800
H	1.63326100	1.36053400	3.37837900
H	1.39145500	-1.87489300	3.15415100
H	-0.13539300	-3.62843100	0.83544600
H	-1.72665200	-2.66641600	-1.82369700
H	-2.23938600	0.40464200	-2.90567100

H	-1.35882400	3.12946400	-1.44328200
H	1.22647200	6.16732700	2.66559600
H	3.01519000	1.76046800	6.08149500
H	2.37631000	-4.02990800	5.09850800
H	-0.33200600	-6.68247900	0.59337200
H	-3.20300400	-4.32046000	-3.94322900
H	-3.93837500	1.35698100	-5.26987500
H	-1.76754100	6.02521300	-2.37453400
H	-3.25529400	4.31694300	-0.33845400
H	-1.18463800	4.35517500	3.09960900
H	0.11679300	1.20464100	5.31501100
H	-0.35762600	-2.74490900	4.70120900
H	-2.26401600	-4.59562600	1.68748600
H	-4.16774000	-2.93244400	-1.40743900
H	-4.48054600	1.09603000	-2.28205300
H	-2.49673000	7.23661100	-0.11835100
H	0.48598300	5.69161200	5.22982500
H	1.68675000	-0.01307400	7.59203500
H	0.28238000	-5.65507400	5.22071400
H	-2.92086000	-7.00606600	-0.01227900
H	-5.53553200	-2.97642900	-4.10382100
H	-5.32206500	3.32272800	-4.13882700
H	-0.42212200	6.54434900	-0.73022100
H	2.27829700	4.90185100	4.07096200
H	3.27712700	-0.46195300	6.05415300
H	1.75571500	-5.45285200	3.51742900
H	-1.23805500	-6.29674000	-1.35936500
H	-3.50999400	-2.39743000	-4.95641800
H	-3.15625500	3.41110000	-4.76064900
C	14.26880100	0.56735900	-3.49307200
C	13.03717700	0.50853600	-2.92330300
C	11.75243800	0.44749700	-3.58562400
C	10.56879500	0.39520700	-2.91293300
C	9.24380800	0.33253100	-3.49629500
C	8.16004500	0.28577900	-2.65311200
C	6.77000400	0.22227800	-2.99999700
C	5.76959200	0.17965000	-2.06724400
C	4.35206300	0.11006300	-2.33025500
C	3.49792600	0.05701200	-1.24929300
C	2.07295400	-0.04147800	-1.29138600
C	1.23823700	-0.04217100	-0.19896700
C	-0.18340100	-0.13896500	-0.32694800
C	-1.14592600	-0.07764800	0.65861000
C	-2.52924800	-0.14268200	0.25415800
C	-3.63485100	0.01674900	1.04718100
C	-4.96277500	0.01748600	0.50230900
C	-6.15839500	0.24070400	1.14095100
C	-7.36427100	0.28263800	0.33586000
C	-8.63854900	0.46522300	0.78375100
C	-9.78706900	0.51609800	-0.09489600
C	-11.09112100	0.68972500	0.24344100
H	12.99590100	0.50837900	-1.82697000
H	10.60421100	0.39968800	-1.81668700
H	8.37543000	0.29855500	-1.57783000
H	6.05705100	0.19374600	-1.00938100
H	3.96196400	0.09319800	-0.25977300
H	1.67674600	0.05162200	0.79556400
H	-9.56152000	0.40183000	-1.16257500
H	-7.21300900	0.18413800	-0.74672600
H	-5.01880300	-0.16969800	-0.57543500
H	-2.70089500	-0.31539100	-0.81388900
H	-0.54670700	-0.25710200	-1.35184500
H	1.60533000	-0.11757300	-2.27341300
H	11.74005500	0.44126200	-4.67828100
H	6.50235000	0.20551600	-4.05893100
H	-8.81003900	0.57639400	1.85741600
H	-3.50365300	0.19203700	2.11802500
H	15.21417500	0.78734000	-1.57319900
C	-12.15641600	0.69887200	-0.82989700
C	-14.36698200	-1.28151300	-2.90602000
C	-13.53206400	-2.49797300	-3.22049400
H	-14.15670200	-3.40964700	-3.21605100
H	-12.70329300	-2.65413600	-2.51744100

H	-13.10518100	-2.42238300	-4.23681700
C	-15.49759300	-1.03424600	-3.87554900
H	-16.18710100	-1.89756400	-3.90989000
H	-15.11596600	-0.90237800	-4.90450500
H	-16.08144800	-0.14043400	-3.60958700
C	-14.16522300	-0.46009500	-1.85984000
C	-13.09914100	-0.53276600	-0.80091200
C	-11.57751400	0.87555100	1.65768900
H	-12.20384800	1.78256700	1.73430700
H	-10.76318300	0.96722400	2.38824100
H	-12.21569100	0.03239400	1.97706000
C	-6.27404000	0.46160100	2.62863700
H	-6.72835500	1.44254900	2.85101700
H	-5.30327300	0.41670900	3.13819900
H	-6.92738900	-0.29964100	3.08908400
C	-0.82365400	0.09338500	2.12097100
H	-1.17495600	1.07099200	2.49515700
H	0.25095000	0.02937700	2.32346400
H	-1.32433000	-0.68017900	2.72699300
C	3.87952000	0.09883400	-3.76377200
H	2.78936100	0.15804700	-3.86205400
H	4.21772200	-0.81566000	-4.28091400
H	4.30477300	0.95335800	-4.31595000
C	9.12175000	0.32249400	-5.00014300
H	8.08042300	0.27736000	-5.34143900
H	9.65387100	-0.54255600	-5.43163300
H	9.57903900	1.22655100	-5.43733800
C	14.50959400	0.58986800	-4.98055600
H	13.58529400	0.66028400	-5.56861000
H	15.04659300	-0.31585800	-5.31445400
H	15.15041700	1.44725900	-5.25475300
C	15.50397700	0.61051000	-2.62155900
C	16.37068000	-0.67457000	-2.68251500
C	17.60654300	-0.57022300	-1.83121200
C	17.95236200	-1.30526800	-0.75880500
C	17.13417200	-2.43781800	-0.18984100
H	17.70891600	-3.38154800	-0.21167800
H	16.18933200	-2.60645600	-0.72304400
H	16.89523700	-2.24758400	0.87208200
C	19.24417600	-1.03940000	-0.02388600
H	19.89219800	-1.93499000	-0.02315900
H	19.05398600	-0.79482600	1.03719600
H	19.80988400	-0.20828700	-0.47086100
H	16.67627000	-0.84967000	-3.73054500
H	-11.68366900	0.75414000	-1.82372000
H	-12.49277500	-1.44644300	-0.89705200
H	15.74941000	-1.53590400	-2.39309600
H	18.29947400	0.22751900	-2.13140200
H	-13.58686200	-0.58597300	0.18989200
H	-12.77598000	1.61044800	-0.72373300
H	-14.85070900	0.39205300	-1.75733200
H	16.13618200	1.46805300	-2.92350000