**A DFT investigation of the host-guest interactions between boron-based aromatic systems and β-cyclodextrin**

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**Appendix A Supplementary Data:**

1. **Determination of the exchange constant**

In the calculation of the Kexc, we considered for each complex two or three most stable configurations. An example for the Bxb@β-CD complex is shown in Fig.S1.



Fig. S1. Calculated thermodynamic parameters for the three most stable conformers of Bxb@β-CD at the BLYP-D3(BJ)/def2-SVP level of theory.

Table S1. Thermodynamic parameters used for the calculation of exchange constants

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **species** | **Egas (ua)** | **ZPE (ua)** | **Esol (ua)** | **G°gas, 298 (ua)** | **G\*sol, 298  (ua)** |
| PBA | -407.79842 | 0.12042 | -407.81372 | -407.67801 | -407.69331 |
| PhBcat | -637.38646 | 0.17846 | -637.39343 | -637.20800 | -637.21497 |
| PhBpin | -642.12905 | 0.26222 | -642.13770 | -641.86683 | -641.87548 |
| Bxb | -445.85739 | 0.12749 | -445.87033 | -445.72990 | -445.74284 |
| FcBA | -1826.09080 | 0.18601 | -1826,10476 | -1825.90478 | -1825.91875 |
| PBA@β-CD | 3B | -4678.21410 | 1.28581 | -4678.28882 | -4676.92929 | -4677.01502 |
| 0B | -4678.21409 | 1.28580 | -4678.30022 |
| PhBcat@β-CD | -3B | -4907.80196 | 1.34311707 | -4907.88137 | -4906.46009 | -4906.53906 |
| 0B | -4907.80195 | 1.34312444 | -4907.88131 |
| 1A | -4907.80281 | 1.34342239 | -4907.88085 |
| PhBpin@β-CD | -4B | -4912.55174 | 1.42865902 | -4912.62064 | -4911.12315 | -4911.19821 |
| 2A | -4912.54855 | 1.42780402 | -4912.62601 |
| Bxb@β-CD | -5A | -4716.27061 | 1.2919649 | -4716.35255 | -4714.97885 | -4715.06565 |
| -4A | -4716.26842 | 1.29181053 | -4716.35746 |
| 1B | -4716.26954 | 1.29285748 | -4716.35289 |
| BA@β-CD | -4B | -4522.61950 | 1.21184319 | -4522.70606 | -4521.40786 | -4521.49668 |
| -1B | -4522.61703 | 1.21139082 | -4522.70729 |
| FcBA@β-CD | 0A | -6096.51154 | 1.35112691 | -6096.59514 | -6095.16105 | -6095.24561 |
| -2A | -6096.51153 | 1.35114447 | -6096.59656 |

1. **RDG-isosurfaces of the six studied complexes**



**Fig. S2.** RDG-isosurfaces of isolated β-CD and studied aromatic boron compounds computed at BLYP-D3(BJ) level. Atom's color code: pink for B, purple for Fe, blue for C, red for O and white for H.

1. Supplementary structures

**Table S2.** Cartesian coordinates (in angstrom) of aromatic boron compounds and their complexes optimized at BLYP-D3(BJ)/def2-SVP level of theory in vacuum and aqueous solution

|  |  |  |
| --- | --- | --- |
| **Species** | **Geometries in gas phase** | **Geometries in aqueous solution** |
| **PBA** | B -0.20932 -0.17441 3.38451C -0.02174 0.01350 4.94054C -0.70370 1.04390 5.64429C -0.53852 1.21367 7.03341C 0.31667 0.35147 7.75280C 1.00299 -0.67958 7.07551C 0.83388 -0.84365 5.68640O -1.07036 0.69044 2.72574O 0.49623 -1.19523 2.76519H -1.37342 1.72334 5.08911H -1.07612 2.02177 7.56043H 0.44936 0.48475 8.84143H 1.67225 -1.35752 7.63455H 1.37458 -1.65276 5.16568H -1.16772 0.53914 1.76389H 0.35373 -1.28382 1.80111 | B -0.20931 -0.17453 3.37641C -0.02050 0.01463 4.93930C -0.70320 1.04380 5.64647C -0.53970 1.21361 7.03720C 0.31668 0.35151 7.75770C 1.00490 -0.67862 7.07874C 0.83568 -0.84121 5.68791O -1.06332 0.69237 2.71795O 0.48822 -1.19843 2.76025H -1.37484 1.72573 5.09585H -1.07909 2.02052 7.56414H 0.44800 0.48398 8.84647H 1.67491 -1.35672 7.63662H 1.38004 -1.65134 5.17179H -1.15451 0.52592 1.75444H 0.33482 -1.27622 1.79337 |
| **PhBcat** | C 0.75596 -0.42178 7.07404C -0.08456 0.71471 7.14193C -0.24111 -0.06482 3.49021C 0.38754 -1.07390 2.70785C -1.11139 0.84997 2.83292C -1.34712 0.75753 1.44804C -0.71486 -0.25220 0.69019C 0.15507 -1.16715 1.32222B 0.00807 0.02893 5.01854O -0.55498 1.00539 5.86639O 0.82282 -0.85590 5.75502C 1.37489 -0.95374 8.21149C 1.11928 -0.29483 9.44058C -0.34207 1.37333 8.35034C 0.28029 0.84257 9.50819H 1.06590 -1.79484 3.19686H -1.60950 1.64147 3.41930H -2.02723 1.47362 0.95402H -0.90285 -0.32750 -0.39557H 0.65097 -1.95681 0.73095H 2.02393 -1.84214 8.14796H 1.58497 -0.67967 10.36341H -0.99580 2.25953 8.39243H 0.10456 1.32851 10.48278 | C 0.75400 -0.42301 7.07807C -0.08156 0.71608 7.14489C -0.24130 -0.06524 3.48930C 0.39144 -1.07202 2.70507C -1.11598 0.84740 2.83221C -1.35200 0.75512 1.44637C -0.71543 -0.25224 0.68691C 0.15895 -1.16502 1.31841B 0.00803 0.02859 5.01792O -0.55135 1.00791 5.86613O 0.81936 -0.85891 5.75639C 1.37163 -0.95843 8.21501C 1.11778 -0.29658 9.44424C -0.33809 1.37837 8.35190C 0.28269 0.84507 9.51086H 1.07397 -1.79294 3.18861H -1.61947 1.63819 3.41521H -2.03511 1.46898 0.95357H -0.90309 -0.32703 -0.39880H 0.65821 -1.95208 0.72676H 2.01746 -1.84953 8.15417H 1.58208 -0.68300 10.36710H -0.98794 2.26752 8.39510H 0.10852 1.33308 10.48469 |
| **PhBpin** | C 0.21840 0.15725 -1.49224C 1.50734 0.47346 -2.00257C 1.72080 0.64417 -3.38454C 0.64591 0.49654 -4.28750C -0.64130 0.17877 -3.80244C -0.85028 0.01364 -2.41912B -0.01846 -0.02208 0.04494O -1.25108 -0.34159 0.59334C -1.14128 -0.21329 2.05774C -1.96739 -1.33884 2.71394C -1.73733 1.16727 2.43567O 0.98304 0.12638 0.99219C 0.44472 -0.31216 2.29255C 0.99854 0.61674 3.39265C 0.94567 -1.76112 2.52343H 2.35184 0.58936 -1.30098H 2.72748 0.89537 -3.76266H 0.81191 0.63173 -5.37122H -1.48382 0.06145 -4.50671H -1.85931 -0.23224 -2.04473H -1.67594 -2.34097 2.34023H -1.84595 -1.32569 3.82036H -3.04727 -1.19628 2.48849H -2.78058 1.22970 2.05782H -1.76000 1.31669 3.53686H -1.16494 2.00410 1.98216H 0.80174 1.68614 3.17395H 0.54946 0.37051 4.38036H 2.09962 0.48710 3.47916H 2.05604 -1.77638 2.46730H 0.64642 -2.14391 3.52352H 0.55920 -2.46202 1.75249 | C 0.21900 0.15777 -1.49601C 1.50913 0.47111 -2.00878C 1.72328 0.64165 -3.39183C 0.64695 0.49687 -4.29540C -0.64177 0.18219 -3.80917C -0.85034 0.01729 -2.42448B -0.01839 -0.02193 0.04410O -1.24970 -0.34565 0.58950C -1.14109 -0.21393 2.06491C -1.96422 -1.33982 2.72082C -1.73776 1.16658 2.43591O 0.98263 0.13167 0.98903C 0.44250 -0.31286 2.29927C 0.99369 0.61641 3.39833C 0.94595 -1.76034 2.52340H 2.35843 0.58609 -1.31243H 2.73070 0.89022 -3.76920H 0.81256 0.63149 -5.37906H -1.48514 0.06724 -4.51261H -1.86219 -0.22587 -2.05519H -1.67110 -2.34254 2.34929H -1.83511 -1.32268 3.82572H -3.04570 -1.19566 2.50309H -2.78341 1.22571 2.06322H -1.75762 1.31469 3.53673H -1.16608 2.00393 1.98197H 0.79684 1.68611 3.17990H 0.53620 0.36884 4.38110H 2.09356 0.48164 3.49394H 2.05698 -1.77359 2.47361H 0.64458 -2.14164 3.52276H 0.55985 -2.46120 1.75195 |
| **Bxb** | C -0.77268 1.86885 6.28432C -0.18419 1.33792 7.45287C -0.64440 1.14754 5.08195C 0.05853 -0.08703 5.02653C 0.64097 -0.60430 6.20573C 0.51815 0.10934 7.41621H -1.31750 2.82889 6.32223H -0.27217 1.88641 8.40708H 1.19053 -1.56391 6.19277H 0.96950 -0.28765 8.34192C -1.18157 1.49213 3.69776O -0.76760 0.42349 2.81603B -0.04270 -0.53387 3.51809O 0.43625 -1.63308 2.84736H -0.77988 2.46263 3.31665H -2.29658 1.57116 3.68521H 0.92433 -2.24400 3.43440 | C -0.77462 1.87136 6.28367C -0.18542 1.33921 7.45252C -0.64494 1.14843 5.08116C 0.05929 -0.08662 5.02824C 0.64325 -0.60655 6.20709C 0.51865 0.10940 7.41710H -1.31996 2.83070 6.31888H -0.27403 1.88762 8.40676H 1.19165 -1.56577 6.18871H 0.96962 -0.28555 8.34389C -1.18365 1.49768 3.70106O -0.76483 0.42024 2.81495B -0.03867 -0.53640 3.52618O 0.43505 -1.63201 2.84642H -0.78021 2.46528 3.31880H -2.29749 1.57242 3.68715H 0.92530 -2.25492 3.42451 |
| **FcBA** | Fe 0.00010 0.00246 5.00003C 1.06795 -0.33767 3.24157C -0.27357 -0.89586 3.14026H -0.50242 -1.95940 2.97663C -1.23702 0.16182 3.30839H -2.33220 0.05146 3.29332C -0.51395 1.39489 3.51688H -0.95951 2.38737 3.68301C 0.89551 1.09172 3.47710H 1.69975 1.83458 3.60594C 1.24905 -0.25205 6.65002H 2.34906 -0.22049 6.62082C 0.43384 -1.43124 6.45030H 0.80538 -2.44611 6.24337C -0.95208 -1.03567 6.54718H -1.82282 -1.69912 6.43531C -0.99500 0.38609 6.80313H -1.90374 0.99445 6.92439C 0.36539 0.87047 6.86805H 0.67154 1.91199 7.04811B 2.39776 -1.16202 3.32212O 3.62445 -0.61225 3.67927H 3.56770 0.33841 3.90171O 2.35529 -2.51522 3.04683H 3.23514 -2.93350 3.16230 | Fe -0.00058 -0.00028 4.99861C 1.06641 -0.34142 3.24096C -0.27796 -0.89992 3.14197H -0.51630 -1.96256 2.98214C -1.24066 0.16064 3.30885H -2.33636 0.05160 3.29512C -0.51405 1.39354 3.51438H -0.95847 2.38682 3.68133C 0.89600 1.08968 3.47468H 1.70530 1.82595 3.60724C 1.25181 -0.24859 6.64720H 2.35162 -0.21177 6.61226C 0.43642 -1.42987 6.45211H 0.80858 -2.44585 6.24934C -0.95117 -1.03498 6.54921H -1.82220 -1.69916 6.43988C -0.99444 0.38852 6.80215H -1.90353 0.99703 6.92231C 0.36695 0.87407 6.86420H 0.67383 1.91665 7.03813B 2.40031 -1.16008 3.32279O 3.61861 -0.60954 3.69954H 3.56148 0.33656 3.95000O 2.36573 -2.50849 3.01289H 3.23827 -2.94347 3.13871 |
| **PBA@β-CD** | C 5.72897 -2.99410 0.23050C 6.43020 -2.16484 1.33764C 5.91622 -0.71183 1.35048C 5.91633 -0.07324 -0.06597C 5.32491 -1.03255 -1.14495C 5.54207 -0.55539 -2.58556C 1.21113 -5.94698 0.50286C 2.14643 -5.92892 1.73926C 2.98892 -4.63765 1.78897C 3.68941 -4.40160 0.42676C 2.66113 -4.42723 -0.73662C 3.25461 -4.22858 -2.16050C -3.96499 -4.59484 -0.03120C -3.50196 -5.42877 1.19721C -2.03108 -5.12693 1.55037C -1.15656 -5.30763 0.28760C -1.67948 -4.42366 -0.87553C -0.89127 -4.57356 -2.20761C -6.43662 0.23176 0.24286C -6.82573 -0.84556 1.29213C -5.69878 -1.88845 1.46232C -5.24426 -2.46297 0.09358C -4.95818 -1.31026 -0.91721C -4.67457 -1.80846 -2.34007C -3.84674 4.86348 1.15088C -4.55495 4.26037 2.38937C -4.74224 2.73830 2.23075C -5.43602 2.41851 0.88537C -4.74598 3.13207 -0.31542C -5.50554 2.99196 -1.64374C 1.39825 5.71147 0.32820C 0.72787 6.18702 1.64398C -0.50857 5.32810 1.97278C -1.45011 5.27311 0.74506C -0.69334 4.79992 -0.52470C -1.55967 4.74279 -1.81435C 5.50855 2.35345 -0.50177C 5.59277 3.42422 0.62558C 4.19282 3.79035 1.16020C 3.26292 4.14442 -0.02345C 3.22420 2.97799 -1.04622C 2.30688 3.21881 -2.27450O 6.22647 -2.81158 2.61009O 6.73003 0.01876 2.27302O 5.10076 1.11122 0.06714O 5.94230 -2.35408 -1.03580O 4.79307 -1.41642 -3.46014O 1.35398 -6.10434 2.92961O 3.91392 -4.78806 2.87104O 4.34493 -3.11144 0.53186O 1.97907 -5.73532 -0.69627H 3.19094 -3.14844 -2.42435O 4.58765 -4.72043 -2.33080O -4.38217 -5.18794 2.31434O -1.66854 -6.01577 2.61267O 0.20064 -4.95954 0.65500O -3.08239 -4.79775 -1.13191O -0.41981 -5.89063 -2.49998O -7.12512 -0.19780 2.54467O -6.19702 -2.89525 2.34461O -4.03655 -3.21499 0.33698O -6.10393 -0.41326 -0.99658O -3.93332 -0.78925 -3.09065O -3.79627 4.59207 3.56878O -5.50477 2.28985 3.35796O -5.33558 0.98136 0.73675O -4.60001 4.56771 -0.03714O -6.89269 3.32502 -1.45378O 1.70114 6.16069 2.70469O -1.13043 5.90799 3.12542O -2.52303 4.35427 1.06898O 0.43780 5.71638 -0.74618O -2.54291 5.77304 -1.95010O 6.45853 2.94890 1.67869O 4.36972 4.87492 2.07958O 1.95256 4.42012 0.52726O 4.60204 2.77039 -1.51966O 2.31374 4.54576 -2.80614H 6.20034 -4.00011 0.14135H 7.52160 -2.14592 1.08750H 4.84920 -0.73269 1.68796H 6.96718 0.20051 -0.33503H 4.22793 -1.11525 -0.96805H 6.64041 -0.58188 -2.81463H 5.19750 0.50516 -2.66015H 0.75754 -6.95920 0.38478H 2.85535 -6.78830 1.62036H 2.29353 -3.77569 1.96591H 4.44827 -5.19719 0.24275H 1.89473 -3.63624 -0.56448H -4.96381 -4.95379 -0.37844H -3.56306 -6.50700 0.89953H -1.95232 -4.05563 1.87251H -1.19638 -6.37147 -0.04593H -1.64595 -3.34867 -0.58200H -0.06716 -3.82021 -2.20413H -1.58605 -4.27282 -3.02680H -7.29800 0.89686 0.00512H -7.73512 -1.37445 0.90648H -4.80868 -1.36438 1.89849H -6.04894 -3.13185 -0.30531H -4.06972 -0.74846 -0.54477H -5.64511 -2.02572 -2.84395H -4.07607 -2.74671 -2.29789H -3.83785 5.97673 1.22043H -5.57140 4.72746 2.44257H -3.73047 2.25682 2.20940H -6.50383 2.73190 0.94280H -3.73908 2.67576 -0.45470H -5.38311 1.93874 -2.00046H -5.01103 3.66755 -2.38816H 2.18594 6.43774 0.01838H 0.37919 7.23761 1.47017H -0.16202 4.28449 2.18399H -1.86588 6.28849 0.54375H -0.28502 3.77991 -0.34495H -2.00780 3.72162 -1.86626H -0.85995 4.82675 -2.67899H 6.50176 2.24978 -1.00145H 6.03102 4.34757 0.16701H 3.75771 2.89305 1.67171H 3.65037 5.04820 -0.55137H 2.87150 2.04724 -0.54204H 1.27778 2.88173 -1.99439H 2.65559 2.52859 -3.07790H 6.54761 -2.18043 3.29296H 6.49014 0.97928 2.20340H 4.89455 -1.08439 -4.37601H 1.95206 -5.91200 3.68674H 4.53657 -4.01736 2.86559H 5.17145 -3.92727 -2.31269H -3.92471 -5.56733 3.09972H -0.71089 -5.87748 2.82553H 0.46994 -5.97939 -2.08163H -7.21771 -0.92499 3.20236H -5.50159 -3.59619 2.45318H -4.22277 -0.81629 -4.02644H -4.16616 4.04527 4.29789H -5.84349 1.37942 3.16456H -7.33131 3.29221 -2.32902H 1.19411 6.28230 3.53940H -1.91314 5.35307 3.37425H -3.34100 5.48631 -1.44565H 6.34419 3.58746 2.41995H 3.47880 5.15149 2.41400H 1.65911 5.07328 -2.28848H 2.57713 -4.77089 -2.86420B -1.19993 0.03903 -1.32169C -0.12251 0.21155 -0.18255C -0.25950 1.20669 0.82417C 0.67906 1.32131 1.87035C 1.76921 0.42917 1.94201C 1.91963 -0.57512 0.96117C 0.98751 -0.67245 -0.09058O -2.19726 0.99926 -1.45451O -1.14128 -1.08210 -2.13352H -1.12155 1.89422 0.79565H 0.55556 2.10320 2.63991H 2.50010 0.51010 2.76621H 2.75400 -1.29081 1.02220H 1.11434 -1.45811 -0.85574H -2.89382 0.73016 -2.09866H -1.90977 -1.13208 -2.75060 | C 5.46525 -2.91933 -0.44535C 6.33032 -2.17583 0.61111C 5.78713 -0.75502 0.87603C 5.54441 0.01932 -0.44720C 4.70490 -0.83583 -1.44008C 4.54411 -0.21011 -2.82946C 1.26187 -6.17261 0.39315C 2.30239 -6.10748 1.54761C 3.06076 -4.76626 1.50018C 3.65556 -4.52993 0.09149C 2.58793 -4.70111 -1.02849C 3.15486 -4.64452 -2.45575C -3.90435 -4.59673 0.62534C -3.24374 -5.02844 1.96427C -1.71032 -4.84770 1.92557C -1.12604 -5.52775 0.66226C -1.86125 -5.05961 -0.62650C -1.41624 -5.78765 -1.90315C -6.22469 0.21072 -0.11816C -6.70508 -0.78300 0.97693C -5.57455 -1.76224 1.36456C -4.98350 -2.44407 0.09849C -4.58355 -1.37544 -0.95820C -4.10754 -1.97267 -2.29147C -3.98442 5.05043 0.62938C -4.91303 4.55803 1.77566C -5.00812 3.01735 1.77603C -5.37033 2.49109 0.36552C -4.45191 3.09233 -0.73726C -4.87179 2.73416 -2.17086C 1.35344 5.80268 0.95998C 0.57747 5.92287 2.29739C -0.76373 5.16278 2.23945C -1.56732 5.55536 0.97328C -0.70703 5.47770 -0.32001C -1.40283 6.01649 -1.57853C 5.30226 2.49915 -0.48972C 5.42257 3.42397 0.75860C 4.02845 3.71300 1.35252C 3.10271 4.25421 0.23563C 3.04507 3.27045 -0.96025C 2.14683 3.73946 -2.13124O 6.37239 -2.97050 1.81698O 6.72913 -0.08674 1.72960O 4.83320 1.22355 -0.07201O 5.36877 -2.12682 -1.62888O 3.51868 -0.92615 -3.54117O 1.61466 -6.30005 2.80391O 4.07842 -4.78435 2.51578O 4.18029 -3.18295 0.11030O 1.92057 -5.99641 -0.86455H 3.47281 -3.59670 -2.66454O 4.25012 -5.57065 -2.60209O -3.84963 -4.27325 3.03641O -1.17480 -5.40832 3.13454O 0.27427 -5.16479 0.61070O -3.30188 -5.28350 -0.47356O -1.52382 -7.21274 -1.73000O -7.17599 -0.03031 2.11504O -6.12550 -2.70943 2.29276O -3.79774 -3.17874 0.48143O -5.73055 -0.51898 -1.24793O -3.13337 -1.07472 -2.89922O -4.40888 5.07286 3.02794O -5.98803 2.63667 2.75545O -5.21717 1.05258 0.43110O -4.45355 4.55366 -0.62559O -6.25444 3.07774 -2.38704O 1.43945 5.44155 3.35013O -1.48884 5.46129 3.44287O -2.65427 4.60512 0.89607O 0.53745 6.23820 -0.14526O -1.84886 7.36710 -1.36053O 6.30815 2.80993 1.71868O 4.19202 4.65728 2.42738O 1.77968 4.45919 0.78671O 4.41542 3.09060 -1.45315O 2.26076 5.12923 -2.48418H 5.95920 -3.86748 -0.75969H 7.36043 -2.07996 0.18326H 4.79142 -0.84833 1.37800H 6.52832 0.28055 -0.90934H 3.69067 -0.99432 -1.00240H 5.53231 -0.25499 -3.35785H 4.28121 0.86820 -2.70684H 0.79175 -7.18148 0.34375H 3.03459 -6.93796 1.38672H 2.32036 -3.95160 1.70028H 4.47872 -5.26133 -0.08337H 1.83308 -3.88304 -0.94201H -4.97360 -4.90981 0.61717H -3.45815 -6.11848 2.09359H -1.48699 -3.75112 1.85598H -1.23375 -6.63384 0.75860H -1.66279 -3.97026 -0.77134H -0.36716 -5.48198 -2.12388H -2.05674 -5.42561 -2.74877H -7.07821 0.81291 -0.50555H -7.54726 -1.37685 0.53882H -4.74882 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-4.93475 4.65184 3.74606H -6.19359 1.67322 2.62581H -6.52649 2.66551 -3.23502H 0.92486 5.45638 4.18835H -2.41545 5.11889 3.33505H -2.48743 7.58193 -2.07412H 6.19270 3.30153 2.56463H 3.31203 4.76617 2.87050H 1.75645 5.65130 -1.81422H 2.31968 -4.88612 -3.16345B -0.62909 -0.30330 -0.81127C 0.34735 -0.06822 0.41275C 0.39628 1.18366 1.08736C 1.22832 1.38293 2.20890C 2.03849 0.32599 2.67958C 2.01081 -0.92487 2.02496C 1.17521 -1.11515 0.90506O -1.49862 0.72133 -1.16377O -0.60549 -1.51965 -1.47348H -0.23457 2.01357 0.72703H 1.25299 2.36535 2.70931H 2.69351 0.47767 3.55529H 2.64418 -1.75182 2.38695H 1.14840 -2.09858 0.40882H -2.11811 0.44910 -1.88334H -1.31747 -1.56550 -2.16229 |
| **PhBcat@β-CD** | C 2.77726 -5.73358 -0.71415C 3.79592 -5.57756 0.44441C 4.19017 -4.09939 0.64315C 4.63995 -3.45375 -0.69583C 3.60317 -3.73502 -1.82514C 4.05072 -3.26526 -3.21375C -2.60725 -5.74809 -0.48170C -1.81140 -6.45810 0.64327C -0.40570 -5.84293 0.80222C 0.30746 -5.79723 -0.57220C -0.56276 -5.07567 -1.63644C 0.05015 -5.03578 -3.06610C -6.12807 -1.69822 -0.23683C -6.20096 -2.83481 0.82266C -4.81921 -3.48706 1.02975C -4.22804 -3.90102 -0.33836C -4.19065 -2.69502 -1.31415C -3.64139 -3.02357 -2.73163C -5.18157 3.52984 0.83007C -5.86339 2.71369 1.95845C -5.57875 1.20611 1.80656C -5.90593 0.71255 0.37202C -5.25791 1.63957 -0.70109C -5.67096 1.32144 -2.14278C -0.36154 5.93907 0.85731C -1.19484 5.91461 2.16368C -2.12224 4.68425 2.19000C -2.98362 4.66153 0.90566C -2.07510 4.69493 -0.35658C -2.83366 4.69599 -1.71461C 4.53225 3.83218 0.05634C 4.25098 4.56587 1.39449C 2.74724 4.55086 1.72650C 1.91973 5.04219 0.51482C 2.28479 4.25107 -0.76896C 1.51640 4.69595 -2.04834C 5.91649 -1.30764 -0.78415C 6.46060 -0.59052 0.48470C 5.49734 0.52550 0.93765C 5.21608 1.47603 -0.25057C 4.66657 0.66719 -1.45674C 4.34175 1.50891 -2.72491O 3.23843 -6.14101 1.64746O 5.21184 -4.07682 1.64046O 4.73170 -2.03313 -0.44474O 3.34020 -5.17059 -1.91388O 2.89623 -3.26018 -4.07934O -2.57095 -6.39858 1.86606O 0.28830 -6.64298 1.76403O 1.55977 -5.09596 -0.36453O -1.85971 -5.77397 -1.71074H 0.61314 -4.08287 -3.17774O 0.87181 -6.15840 -3.40274O -6.73516 -2.31110 2.05711O -5.01028 -4.59659 1.91396O -2.90078 -4.41738 -0.08199O -5.56441 -2.18743 -1.45162O -3.98348 -4.31155 -3.24583O -5.42037 3.20992 3.23677O -6.34694 0.53448 2.80675O -5.35487 -0.61876 0.29011O -5.62467 3.03287 -0.44388O -4.73304 1.97127 -3.02690O -0.30615 5.94597 3.29845O -2.88796 4.76818 3.39989O -3.76973 3.44323 0.95536O -1.23808 5.90725 -0.28419O -4.10604 5.35266 -1.69754O 5.03010 3.95306 2.44309O 2.57209 5.35804 2.89468O 0.52778 4.83155 0.85077O 3.73231 4.40117 -0.99784O 1.19131 6.08468 -2.12210O 6.68668 -1.55854 1.53127O 6.10204 1.17796 2.06283O 4.25518 2.44891 0.21784O 5.66055 -0.35456 -1.81413O 5.18107 2.64356 -2.94699H 2.61400 -6.81228 -0.94322H 4.71639 -6.14424 0.14946H 3.27761 -3.54057 0.97922H 5.63982 -3.86668 -0.98051H 2.65879 -3.20575 -1.55944H 4.84455 -3.96100 -3.58998H 4.49590 -2.24560 -3.12343H -3.54557 -6.31319 -0.69650H -1.68010 -7.52443 0.32663H -0.52156 -4.78628 1.15963H 0.50531 -6.83505 -0.92879H -0.74486 -4.02518 -1.30732H -7.15720 -1.35172 -0.49599H -6.89032 -3.61837 0.41659H -4.12996 -2.72538 1.48011H -4.86441 -4.69410 -0.79822H -3.55231 -1.88581 -0.88549H -2.53639 -2.86090 -2.70950H -4.06028 -2.25617 -3.42464H -5.51671 4.59231 0.86573H -6.96728 2.86950 1.85159H -4.47846 1.04570 1.95688H -7.01649 0.68791 0.23940H -4.15246 1.52408 -0.61981H -6.71596 1.69122 -2.30596H -5.66282 0.21450 -2.28791H 0.19877 6.89955 0.77405H -1.83780 6.83209 2.16285H -1.49384 3.76018 2.18020H -3.66107 5.54741 0.87594H -1.39861 3.80796 -0.34307H -2.93380 3.64231 -2.06136H -2.17349 5.21791 -2.44927H 5.59103 3.99221 -0.25569H 4.56639 5.63215 1.26024H 2.44767 3.49255 1.92238H 2.11284 6.12511 0.33094H 2.07115 3.16833 -0.60443H 0.60728 4.05296 -2.13618H 2.16669 4.44694 -2.92069H 6.69147 -1.99791 -1.19691H 7.43320 -0.11361 0.19978H 4.52335 0.05711 1.22788H 6.15693 1.98724 -0.56677H 3.72670 0.15628 -1.14632H 3.26342 1.79650 -2.67288H 4.44470 0.82211 -3.59874H 3.82537 -5.84680 2.38093H 5.56652 -3.15211 1.71255H 3.18006 -2.96337 -4.96908H -1.95709 -6.68497 2.57974H 1.22228 -6.31813 1.83306H 1.80261 -5.85756 -3.28500H -6.59419 -3.02018 2.72623H -4.14145 -5.05962 2.02969H -3.28453 -4.93923 -2.94175H -5.73357 2.55777 3.90428H -6.30299 -0.44319 2.63786H -5.02351 1.81565 -3.94989H -0.86345 5.73420 4.08120H -3.61189 4.09016 3.37218H -4.77876 4.63732 -1.61988H 4.61529 4.24368 3.28811H 1.60975 5.36182 3.13339H 0.29732 6.19257 -1.71954H 6.87186 -1.03475 2.34417H 5.62995 2.03591 2.23107H 4.72850 3.41642 -2.53312H -0.80726 -4.99231 -3.78085C 1.81253 1.12017 2.90319C 0.54396 1.70973 3.11382C 0.07267 0.21935 -0.28113C 0.91153 -0.59704 -1.09194C -1.16351 0.66488 -0.83088C -1.54387 0.31934 -2.14389C -0.68898 -0.48365 -2.93181C 0.53956 -0.94393 -2.40681B 0.51963 0.66941 1.13557O -0.27555 1.41805 2.02769O 1.79969 0.44866 1.68325C 2.86862 1.28691 3.80803C 2.59618 2.07701 4.95323C 0.26382 2.48884 4.24351C 1.32515 2.66238 5.16623H 1.86995 -0.96091 -0.68532H -1.82756 1.30149 -0.21994H -2.49752 0.68893 -2.55776H -0.97819 -0.74768 -3.96382H 1.21184 -1.56158 -3.02738H 3.86641 0.86055 3.62268H 3.39789 2.24193 5.69353H -0.72534 2.94902 4.39563H 1.15607 3.27252 6.06961 | C 2.81767 -5.77320 -0.92807C 3.89031 -5.64698 0.18808C 4.22743 -4.16434 0.46092C 4.55703 -3.40530 -0.85408C 3.47296 -3.67026 -1.93968C 3.81598 -3.09610 -3.31879C -2.53730 -5.83548 -0.25243C -1.68575 -6.44838 0.88823C -0.26579 -5.84907 0.89310C 0.37121 -5.96953 -0.51573C -0.55809 -5.41021 -1.63346C -0.05675 -5.65776 -3.06403C -6.00092 -1.74268 -0.20231C -6.06970 -2.85211 0.88895C -4.68112 -3.48448 1.12378C -4.08678 -3.93234 -0.23409C -4.04671 -2.75322 -1.24067C -3.47717 -3.11622 -2.63669C -5.13700 3.51364 0.76965C -5.79261 2.70570 1.91915C -5.47611 1.20169 1.78963C -5.81556 0.68066 0.36650C -5.20377 1.59609 -0.73612C -5.65283 1.24436 -2.15883C -0.39970 6.07843 0.66293C -1.25432 6.10576 1.96334C -2.13339 4.84131 2.06137C -2.96636 4.68876 0.76626C -2.02985 4.66778 -0.47241C -2.74993 4.53403 -1.84162C 4.53230 3.87018 0.39427C 4.13749 4.51047 1.74864C 2.60700 4.58764 1.88782C 1.96394 5.26351 0.64872C 2.49160 4.66741 -0.69100C 2.05213 5.44263 -1.94104C 5.74127 -1.21230 -0.84419C 6.31023 -0.54829 0.44576C 5.34266 0.52522 0.98965C 5.02465 1.52619 -0.14714C 4.42541 0.77446 -1.36359C 4.03403 1.67833 -2.56068O 3.41166 -6.31431 1.37603O 5.31660 -4.14146 1.39224O 4.59396 -1.99496 -0.51265O 3.28338 -5.10912 -2.10537O 2.63854 -3.15212 -4.15050O -2.38443 -6.23419 2.13132O 0.50049 -6.54611 1.88540O 1.59606 -5.20388 -0.46186O -1.89128 -6.02552 -1.52484H 0.85526 -5.03834 -3.23197O 0.20641 -7.05934 -3.25932O -6.62538 -2.28635 2.09514O -4.85357 -4.58377 2.03163O -2.75720 -4.45369 0.01188O -5.42232 -2.26497 -1.40384O -3.88186 -4.39175 -3.16077O -5.34355 3.25182 3.17631O -6.21757 0.51470 2.80579O -5.23633 -0.64425 0.29368O -5.57854 2.99393 -0.49602O -4.79908 1.93980 -3.08962O -0.38430 6.24933 3.10762O -2.94589 4.97233 3.23934O -3.71984 3.45523 0.88628O -1.25701 5.91819 -0.47367O -4.03111 5.18262 -1.92685O 4.74298 3.74909 2.81746O 2.32743 5.29597 3.10262O 0.54218 5.00895 0.74517O 3.96035 4.62205 -0.69318O 2.44473 6.82135 -1.83141O 6.59561 -1.57283 1.42076O 5.97353 1.14815 2.12005O 4.10128 2.51467 0.36794O 5.41983 -0.20702 -1.81454O 4.95252 2.74018 -2.86408H 2.67343 -6.83927 -1.21878H 4.81560 -6.15384 -0.18491H 3.31674 -3.67957 0.89869H 5.55612 -3.73784 -1.22687H 2.51738 -3.21606 -1.59150H 4.65729 -3.69064 -3.75904H 4.17397 -2.04772 -3.19082H -3.50487 -6.38177 -0.33456H -1.59905 -7.54430 0.67983H -0.34664 -4.75873 1.13963H 0.59038 -7.04160 -0.72761H -0.65075 -4.30677 -1.48947H -7.03019 -1.41554 -0.47788H -6.74964 -3.65200 0.50131H -4.00055 -2.70955 1.56097H -4.73136 -4.73178 -0.67035H -3.41701 -1.92674 -0.83346H -2.36601 -3.02599 -2.58445H -3.82346 -2.33365 -3.35038H -5.49117 4.56940 0.79583H -6.89936 2.83780 1.81926H -4.37221 1.06587 1.93290H -6.92529 0.62996 0.25016H -4.09630 1.49689 -0.67715H -6.72643 1.53855 -2.28443H -5.58066 0.13966 -2.29431H 0.12034 7.05294 0.51388H -1.93048 6.99522 1.89546H -1.46963 3.94519 2.13610H -3.66905 5.54895 0.66308H -1.31598 3.81544 -0.38375H -2.83945 3.45371 -2.09363H -2.07637 4.98973 -2.60535H 5.63450 3.93891 0.24630H 4.54665 5.55265 1.74930H 2.21103 3.54414 1.93631H 2.17137 6.35847 0.67502H 2.09232 3.62866 -0.78190H 0.94474 5.33378 -2.03645H 2.51669 4.94794 -2.83325H 6.52424 -1.84713 -1.32152H 7.26229 -0.03598 0.15489H 4.38558 0.03090 1.29072H 5.96567 2.02566 -0.47772H 3.50141 0.23679 -1.04773H 3.00487 2.06773 -2.36944H 3.96120 1.02452 -3.46079H 4.02573 -6.07070 2.10671H 5.60222 -3.19613 1.51386H 2.82397 -2.63331 -4.96339H -1.78812 -6.52097 2.85954H 1.44899 -6.26176 1.79914H 0.73744 -7.14365 -4.08006H -6.50751 -2.95967 2.80477H -3.96238 -4.98485 2.20257H -3.28026 -5.07238 -2.77131H -5.64381 2.63753 3.88463H -6.15638 -0.46259 2.62946H -5.02739 1.62887 -3.99260H -0.94575 6.12150 3.90699H -3.59688 4.22194 3.25706H -4.70322 4.48897 -1.72107H 4.19169 3.88824 3.62226H 1.34224 5.41035 3.17513H 2.00133 7.30894 -2.55873H 6.80233 -1.11330 2.26704H 5.41815 1.92220 2.40600H 4.72040 3.50324 -2.27988H -0.84552 -5.28528 -3.76900C 1.70980 0.96733 2.90342C 0.51292 1.70599 3.05600C -0.04322 0.16451 -0.30385C 0.74166 -0.71728 -1.10038C -1.25330 0.67160 -0.85928C -1.66073 0.32164 -2.16302C -0.85792 -0.54555 -2.93787C 0.34289 -1.06811 -2.40668B 0.42594 0.61338 1.10539O -0.30082 1.48035 1.94896O 1.65631 0.26516 1.70047C 2.74345 1.02850 3.84569C 2.52701 1.87093 4.96686C 0.28623 2.53699 4.16062C 1.32731 2.60650 5.12078H 1.68059 -1.12893 -0.69260H -1.87450 1.35846 -0.25845H -2.59503 0.73277 -2.58262H -1.16708 -0.81281 -3.96295H 0.97394 -1.73664 -3.01767H 3.68667 0.47613 3.71358H 3.31632 1.95472 5.73385H -0.64573 3.11362 4.27291H 1.19811 3.25400 6.00444 |
| **PhBpin@β-CD** | C -6.34574 -1.21099 -0.57528C -6.48692 -2.46107 0.33117C -5.18806 -3.29265 0.32234C -4.69290 -3.57130 -1.12281C -4.67894 -2.27271 -1.98478C -4.34209 -2.49499 -3.47714C -4.51066 3.74689 0.45671C -5.29461 3.04763 1.59635C -5.20265 1.51339 1.46790C -5.61176 1.07815 0.03797C -4.78757 1.83206 -1.03950C -5.17055 1.51862 -2.51063C 0.41558 5.80171 0.09094C -0.51617 6.18224 1.28110C -1.50555 5.04146 1.60701C -2.22787 4.60843 0.30829C -1.18635 4.19765 -0.76353C -1.76608 3.68269 -2.10029C 5.30594 3.51580 0.39004C 4.91257 4.45231 1.56147C 3.38131 4.58635 1.67343C 2.73648 4.92692 0.30255C 3.24040 3.96051 -0.81172C 2.75729 4.29378 -2.24177C 6.10135 -1.79892 0.28628C 6.48236 -1.08678 1.60885C 5.68721 0.22470 1.76444C 5.80944 1.09263 0.48736C 5.45315 0.28602 -0.79133C 5.61618 1.04839 -2.13719C 2.35844 -5.49881 -0.82333C 3.18889 -5.64748 0.47838C 3.68087 -4.27650 0.98633C 4.39111 -3.51848 -0.16457C 3.45970 -3.39948 -1.40006C 4.05894 -2.65958 -2.63044C -2.92247 -5.23557 -1.69194C 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4.09509 -6.25341 0.21852H 2.78893 -3.66867 1.29341H 5.31001 -4.07340 -0.47018H 2.52824 -2.86151 -1.10040H 3.81886 -1.57286 -2.52312H 3.49418 -3.01855 -3.52343H -3.77078 -5.67269 -2.27092H -2.14302 -7.21472 -1.28282H -1.24610 -4.92040 0.58160H 0.19595 -6.22525 -1.83125H -1.03643 -3.41160 -1.44102H 0.77212 -2.88542 -2.77093H -0.52380 -3.22893 -3.94889H -6.77207 -2.83093 2.22987H -4.66080 -5.09298 0.94969H -3.02949 -1.06382 -3.91542H -5.19372 2.95821 3.55107H -6.11824 -0.02510 2.30876H -6.63937 0.30173 -2.88288H -0.33640 6.62334 3.17679H -3.04679 4.81170 2.82653H -3.66438 4.19123 -2.18770H 5.09658 4.47365 3.50786H 2.14132 5.74978 2.69092H 2.12688 2.66992 -3.21339H 6.33925 -1.45622 3.52536H 5.78686 1.79819 2.95989H 6.20439 2.89969 -2.11692H 2.88579 -6.27537 2.30705H 4.92936 -3.65892 2.39334H 5.93915 -2.19958 -2.34721H -2.90707 -7.11779 0.99080H 0.34383 -6.62502 1.10272H 1.79035 -4.78639 -3.39150H -4.86190 2.40123 -3.12113C -0.05055 0.13186 -1.64496C -1.05467 -0.58093 -0.93546C -0.86557 -0.97309 0.40441C 0.34070 -0.65640 1.06631C 1.35140 0.05657 0.38482C 1.15410 0.44443 -0.95531B -0.22938 0.52665 -3.14740O 0.59299 1.44481 -3.78439C 0.35801 1.34777 -5.25220C 1.51223 0.48519 -5.81813C 0.41695 2.77047 -5.84291O -1.17920 -0.02762 -3.98988C -1.08386 0.63897 -5.32561C -2.27031 1.62651 -5.43293C -1.21257 -0.45827 -6.40204H -1.99971 -0.83561 -1.44145H -1.65981 -1.53124 0.92897H 0.49416 -0.96469 2.11483H 2.29332 0.31556 0.89668H 1.95050 0.99825 -1.48025H 1.51060 -0.54129 -5.39479H 1.45168 0.40291 -6.92430H 2.48361 0.95945 -5.56171H 1.42662 3.20382 -5.67322H 0.23236 2.74388 -6.93919H -0.32700 3.45140 -5.38297H -2.24503 2.42213 -4.66040H -2.28359 2.11899 -6.42898H -3.22456 1.06907 -5.32296H -2.22239 -0.91712 -6.34302H -1.09139 -0.02498 -7.41919H -0.46353 -1.26566 -6.27449 | C -5.97990 -1.00604 -0.66063C -6.16389 -2.16123 0.35808C -4.89067 -3.02787 0.44586C -4.44893 -3.49326 -0.96915C -4.36004 -2.29048 -1.95114C -4.06583 -2.68910 -3.41018C -4.49365 4.09927 0.09427C -5.47218 3.42377 1.09894C -5.25543 1.89456 1.15213C -5.25692 1.31445 -0.28507C -4.20311 2.03925 -1.16253C -4.10879 1.54631 -2.62792C 0.32224 6.22824 1.17224C -0.64501 6.16553 2.38693C -1.71030 5.07137 2.17943C -2.39889 5.22945 0.80175C -1.37650 5.40614 -0.36019C -2.01402 5.77038 -1.70912C 4.94792 3.45969 0.62220C 4.58195 4.01162 2.02532C 3.05711 4.20119 2.16287C 2.50399 5.04620 0.98274C 2.96062 4.45981 -0.38594C 2.58454 5.32052 -1.59815C 5.81667 -1.60726 -0.94586C 6.43562 -1.08492 0.38252C 5.57862 0.05140 0.98308C 5.32814 1.13743 -0.09344C 4.70836 0.52329 -1.37486C 4.47796 1.52731 -2.53501C 2.41554 -5.77210 -1.42583C 3.38766 -5.81338 -0.21468C 3.83674 -4.38971 0.17530C 4.39568 -3.64388 -1.06176C 3.42551 -3.72368 -2.27804C 4.01709 -3.16576 -3.58185C -2.97228 -5.48564 -1.11659C -2.23191 -6.17025 0.06488C -0.78594 -5.64476 0.18950C -0.05629 -5.78785 -1.16944C -0.87943 -5.16908 -2.33774C -0.28767 -5.44335 -3.72879O -6.52676 -1.59728 1.63439O -5.18138 -4.12717 1.31801O -3.13558 -4.09452 -0.83654O 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-1.61811 -1.58997H -4.98623 -3.13403 -3.85392H -3.28033 -3.48155 -3.41345H -4.78743 5.15942 -0.08314H -6.51002 3.60443 0.72021H -4.24885 1.69189 1.60212H -6.25828 1.47539 -0.75135H -3.19108 1.93540 -0.70222H 1.01228 7.09775 1.27540H -1.16529 7.15493 2.43905H -1.19880 4.07623 2.18760H -3.06971 6.11925 0.83420H -0.83152 4.44074 -0.49493H -2.60509 4.89109 -2.05956H -1.18907 5.93702 -2.44863H 6.05277 3.48407 0.48131H 5.06451 5.01832 2.11291H 2.57362 3.19167 2.10824H 2.86989 6.09704 1.08332H 2.50040 3.45008 -0.50618H 3.17894 6.26873 -1.56474H 1.50776 5.59914 -1.51815H 6.52176 -2.30289 -1.45747H 7.44016 -0.65994 0.13110H 4.58666 -0.37086 1.28760H 6.29874 1.60812 -0.37407H 3.72492 0.05454 -1.13309H 3.46027 1.96437 -2.43913H 4.47845 0.92995 -3.47631H 2.19276 -6.80317 -1.78512H 4.29141 -6.39005 -0.53595H 2.93944 -3.82195 0.53466H 5.37236 -4.09958 -1.34637H 2.51132 -3.12539 -2.03873H 4.14884 -2.06425 -3.45458H 3.26690 -3.32525 -4.39914H -3.96351 -5.96834 -1.27988H -2.18020 -7.26216 -0.17408H -0.82351 -4.55430 0.44734H 0.10770 -6.87066 -1.37782H -0.90587 -4.06010 -2.19847H 0.67654 -4.88666 -3.80617H -0.98571 -5.01334 -4.49276H -6.41870 -2.31130 2.30423H -4.35227 -4.66727 1.42183H -2.80663 -1.25331 -3.93852H -5.84811 3.52745 3.02896H -6.19491 0.35350 1.97535H -5.47631 0.22349 -3.09645H -0.50356 5.73728 4.30918H -3.43721 4.59494 3.02604H -3.34664 7.04337 -2.40118H 4.72280 3.38359 3.88877H 1.84178 5.01652 3.50515H 2.65426 5.13290 -3.56481H 6.83889 -1.80639 2.16778H 5.74991 1.30963 2.50693H 5.10958 3.34847 -2.19490H 3.31460 -6.37366 1.67302H 5.24800 -3.63030 1.34781H 5.69441 -3.30870 -4.60008H -2.41623 -6.24599 2.02910H 0.82962 -6.22003 1.19533H 0.43936 -6.97194 -4.72910H -3.65746 2.37637 -3.22212C -0.40695 0.14670 -1.19931C -1.11716 -0.85560 -0.48535C -1.40195 -0.70760 0.88784C -0.98224 0.45158 1.57692C -0.26201 1.45402 0.89031C 0.02301 1.29807 -0.48052B -0.10499 0.06170 -2.73322O 1.01856 0.63963 -3.28734C 0.83537 0.68351 -4.75732C 2.19300 0.44458 -5.44530C 0.31061 2.10506 -5.08255O -0.94400 -0.52848 -3.67860C -0.23599 -0.47904 -4.99973C -1.26034 -0.18189 -6.11109C 0.39200 -1.87705 -5.20546H -1.44407 -1.77402 -1.00032H -1.95385 -1.49957 1.42267H -1.21233 0.57206 2.64989H 0.07743 2.36139 1.41720H 0.58159 2.08711 -1.01361H 2.70310 -0.45846 -5.05332H 2.05537 0.32301 -6.54190H 2.86213 1.31606 -5.28231H 1.00808 2.85056 -4.64281H 0.25223 2.27776 -6.17842H -0.69590 2.28758 -4.64774H -1.84178 0.74099 -5.91124H -0.73729 -0.06065 -7.08460H -1.97767 -1.02413 -6.21248H -0.40871 -2.64707 -5.17205H 0.89525 -1.95322 -6.19255H 1.13457 -2.11865 -4.41595 |
| **Bxb@β-CD** | C -0.33534 6.40493 -2.38806C -1.32056 6.75691 -1.24423C -2.34014 5.62032 -1.02218C -3.01085 5.18040 -2.35193C -1.95587 4.96686 -3.48126C -2.56871 4.72374 -4.86534C 4.40576 3.84707 -2.09220C 4.03327 4.82451 -0.94786C 2.50356 4.96417 -0.81664C 1.88659 5.32079 -2.19114C 2.33095 4.31948 -3.29262C 1.82794 4.66008 -4.72666C 5.57324 -1.39122 -1.87614C 6.22501 -0.38914 -0.88144C 5.30413 0.82295 -0.64007C 4.91708 1.44279 -2.00289C 4.28060 0.38629 -2.94547C 3.95711 0.92512 -4.37115C 2.52136 -5.64153 -0.41015C 3.70160 -5.24842 0.52056C 4.10042 -3.76710 0.33519C 4.32517 -3.42514 -1.16253C 3.12686 -3.91654 -2.01757C 3.32782 -3.79514 -3.53561C -2.70840 -5.28881 0.83561C -1.75341 -5.37552 2.05118C -0.33442 -4.90614 1.67149C 0.16711 -5.64607 0.40574C -0.88713 -5.64495 -0.74336C -0.51640 -6.54414 -1.93339C -5.95809 -1.29763 -0.70327C -5.98021 -1.82140 0.75799C -4.61229 -2.41379 1.15068C -4.19010 -3.46576 0.09673C -4.19447 -2.86275 -1.33355C -3.81549 -3.86884 -2.45590C -5.02102 3.69219 -2.48243C -5.93752 3.48048 -1.24447C -5.59118 2.17001 -0.50735C -5.55274 0.99482 -1.51214C -4.60900 1.31115 -2.70002C -4.52928 0.19193 -3.77594O -0.56992 7.03515 -0.04603O -3.28391 6.08824 -0.05709O -3.67990 3.93522 -2.04584O -1.08743 6.13819 -3.58568O -1.52783 4.25396 -5.74216O 4.64147 4.37171 0.27739O 2.26156 5.96571 0.17706O 0.44850 5.28466 -2.00893O 3.80213 4.28089 -3.32388H 0.87888 4.11165 -4.91630O 1.65716 6.05992 -4.98663O 6.55516 -1.06360 0.35140O 6.02513 1.72906 0.20274O 3.99502 2.53054 -1.74532O 5.22204 -0.73432 -3.08903O 4.88843 1.88064 -4.88542O 3.33789 -5.52042 1.89036O 5.26333 -3.55386 1.13574O 4.43188 -1.98885 -1.25193O 2.87202 -5.33636 -1.76472O 2.13441 -4.17556 -4.25676O -2.30752 -4.59793 3.13016O 0.50299 -5.13660 2.80753O 1.34987 -4.92924 -0.02238O -2.19447 -6.08347 -0.24965O -0.14493 -7.84793 -1.46368O -6.37888 -0.75463 1.63930O -4.75624 -2.96941 2.46360O -2.86338 -3.92961 0.45363O -5.54619 -2.34518 -1.60131O -4.30609 -5.20099 -2.28734O -5.83911 4.62334 -0.36822O -6.57557 2.00207 0.51821O -5.09445 -0.17346 -0.78593O -5.07653 2.55263 -3.33451O -5.75044 -0.50838 -4.02663H 0.30852 7.28202 -2.62954H -1.88405 7.67008 -1.56615H -1.77515 4.72890 -0.64186H -3.75138 5.95891 -2.66037H -1.34036 4.07905 -3.20588H -3.02083 5.68161 -5.23278H -3.38402 3.96649 -4.76531H 5.50511 3.88150 -2.27739H 4.44401 5.82781 -1.22964H 2.08475 3.97187 -0.50359H 2.20808 6.34429 -2.49394H 1.96089 3.30197 -3.02067H 6.31188 -2.17759 -2.16274H 7.16356 -0.01503 -1.36363H 4.36560 0.46586 -0.14238H 5.83323 1.83447 -2.50532H 3.33345 0.00193 -2.49473H 2.91412 1.32322 -4.36316H 3.94931 0.04789 -5.05862H 2.34062 -6.74123 -0.38891H 4.57777 -5.88272 0.22883H 3.24414 -3.13144 0.68275H 5.27050 -3.91296 -1.50957H 2.23128 -3.31962 -1.72779H 4.19964 -4.42004 -3.85493H 3.54493 -2.74116 -3.80656H -3.69339 -5.74562 1.08827H -1.69289 -6.45470 2.34372H -0.38588 -3.81351 1.42425H 0.41844 -6.69722 0.67664H -0.97164 -4.60044 -1.12713H 0.32251 -6.04390 -2.48140H -1.39948 -6.57629 -2.62236H -6.99085 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-3.49392 1.11751O 4.54131 -2.00214 -1.27599O 2.94827 -5.34887 -1.67697O 2.11907 -3.99447 -4.19735O -2.26573 -4.47708 3.15388O 0.60480 -5.04904 2.87134O 1.46671 -4.86910 0.08518O -2.08174 -6.00041 -0.20377O -0.10298 -7.75580 -1.46443O -6.58820 -0.92681 1.54316O -4.83454 -3.04920 2.43158O -2.80908 -3.86428 0.50287O -5.48976 -2.42488 -1.65797O -4.11132 -5.17944 -2.33866O -5.70159 4.53459 0.07464O -6.42640 1.86515 0.85715O -5.20364 -0.23573 -0.81586O -5.42754 2.70114 -3.11820O -6.68088 0.25683 -4.07544H 0.24221 7.13656 -2.74695H -1.89121 7.57361 -1.56865H -1.75690 4.64757 -0.58756H -3.80796 5.88612 -2.53217H -1.48163 3.93005 -3.17141H -3.24635 5.56730 -5.10098H -3.62274 3.87071 -4.61166H 5.49821 3.86366 -2.20592H 4.35135 5.65606 -0.99069H 1.97672 3.71218 -0.62116H 2.15702 6.31954 -2.27656H 1.99581 3.37861 -3.24331H 6.40560 -2.23771 -2.20628H 7.26936 -0.03906 -1.52846H 4.50684 0.49089 -0.24486H 5.86005 1.82477 -2.69489H 3.41414 -0.07965 -2.58391H 3.14400 1.44617 -4.41201H 3.64413 -0.15642 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4.15935 -5.05713 2.53310H 5.72622 -2.56754 0.92182H 1.87691 -4.94571 -4.23186H -1.67976 -4.52624 3.94186H 1.54603 -4.95387 2.56776H 0.29933 -8.22474 -2.22701H -6.45331 -1.23761 2.46832H -3.93863 -3.33511 2.74398H -3.52679 -5.64303 -1.69024H -6.07097 4.24611 0.94132H -6.29644 0.92884 1.16778H -6.81299 -0.57145 -4.58418H 2.50774 4.31508 -5.48862C -1.09423 0.95077 -2.12466C -1.23714 0.01886 -1.07250C -0.44597 0.53617 -3.30655C 0.06091 -0.78569 -3.45270C -0.09453 -1.70746 -2.38978C -0.74143 -1.30189 -1.20196H -1.49575 1.97205 -2.01544H -1.75168 0.32005 -0.14409H 0.28086 -2.73898 -2.49304H -0.88298 -2.01384 -0.37178C -0.17302 1.33695 -4.57109O 0.47278 0.42544 -5.49959B 0.66803 -0.82929 -4.90750O 1.30492 -1.79314 -5.63668H 0.51133 2.19768 -4.37794H -1.08751 1.76852 -5.03802H 1.49404 -2.64200 -5.14593 |
| **FcBA@β-CD** | C 4.15375 4.72185 0.11145C 3.62114 5.66432 1.21844C 2.11157 5.44061 1.46059C 1.29854 5.48218 0.13300C 1.98226 4.60647 -0.96640C 1.37609 4.81247 -2.35690C 6.19383 -0.18486 0.94460C 6.13263 0.72465 2.19513C 5.04035 1.80062 2.04064C 5.22616 2.56130 0.70667C 5.38323 1.59650 -0.50794C 5.72463 2.30831 -1.82582C 3.69309 -4.85665 0.00031C 4.32723 -4.58620 1.39519C 4.35350 -3.07727 1.70949C 5.05709 -2.33576 0.55209C 4.39597 -2.66420 -0.81168C 5.12290 -2.01814 -2.02951C -1.52948 -6.07609 -0.78063C -0.76539 -6.70753 0.40939C 0.43139 -5.83035 0.82809C 1.32670 -5.50995 -0.39942C 0.48471 -4.94694 -1.58623C 1.30405 -4.78953 -2.88621C -5.69376 -2.65421 -0.52951C -5.65076 -3.81387 0.50612C -4.20472 -4.30445 0.71987C -3.54087 -4.63714 -0.63452C -3.69318 -3.47836 -1.65160C -3.18339 -3.82185 -3.08883C -5.39528 2.55703 0.94666C -5.69776 1.54323 2.07747C -5.20257 0.12223 1.73433C -5.71010 -0.30739 0.33647C -5.42505 0.79210 -0.73368C -6.02401 0.47859 -2.11315C -1.13667 5.86617 0.52257C -1.84533 5.67585 1.89671C -2.52620 4.29682 1.98731C -3.48148 4.11903 0.78828C -2.75673 4.37906 -0.56041C -3.72025 4.38244 -1.79116O 4.36436 5.45589 2.43604O 1.71286 6.44557 2.39468O -0.03240 4.95986 0.37999O 3.39355 4.93939 -1.07903O 1.88598 3.78725 -3.24869O 5.92040 -0.09471 3.36203O 5.13330 2.65583 3.18525O 4.03631 3.36800 0.54144O 6.43494 0.61101 -0.23057H 4.81058 2.84995 -2.17096O 6.83218 3.20505 -1.62537O 3.63308 -5.32577 2.41869O 5.03307 -2.93029 2.96176O 4.98124 -0.91708 0.83205O 4.39705 -4.11712 -1.00041O 6.54359 -1.90774 -1.91547O -1.67472 -6.91730 1.50822O 1.11519 -6.55265 1.85373O 2.30379 -4.52464 0.02245O -0.62382 -5.86140 -1.87460O 0.64904 -3.97702 -3.87141O -6.24046 -3.38364 1.75403O -4.27025 -5.43084 1.60128O -2.13435 -4.86315 -0.35932O -5.10728 -3.08625 -1.75220O -3.21130 -5.21509 -3.42799O -5.12066 2.02309 3.30943O -5.65379 -0.72954 2.79112O -4.98984 -1.51314 -0.01059O -5.95310 2.08938 -0.29085O -7.41957 0.16142 -1.98524O -0.92790 5.86323 2.99191O -3.20045 4.26149 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0.07893 2.30697 0.60890B 1.80766 0.01246 -3.25762O 2.70202 1.05945 -3.23839H 2.31272 1.96270 -3.10308O 2.31695 -1.27342 -3.48135H 3.28400 -1.26980 -3.65609 |