**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.

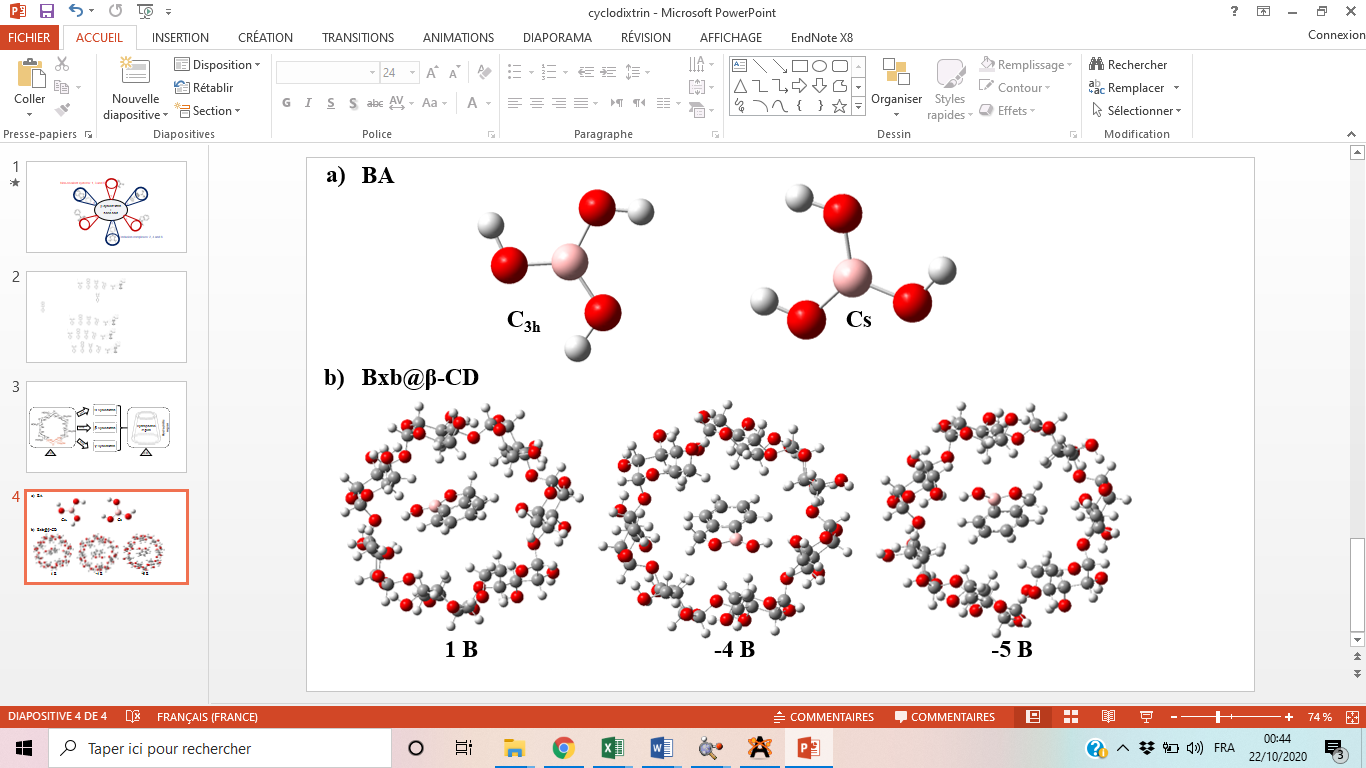
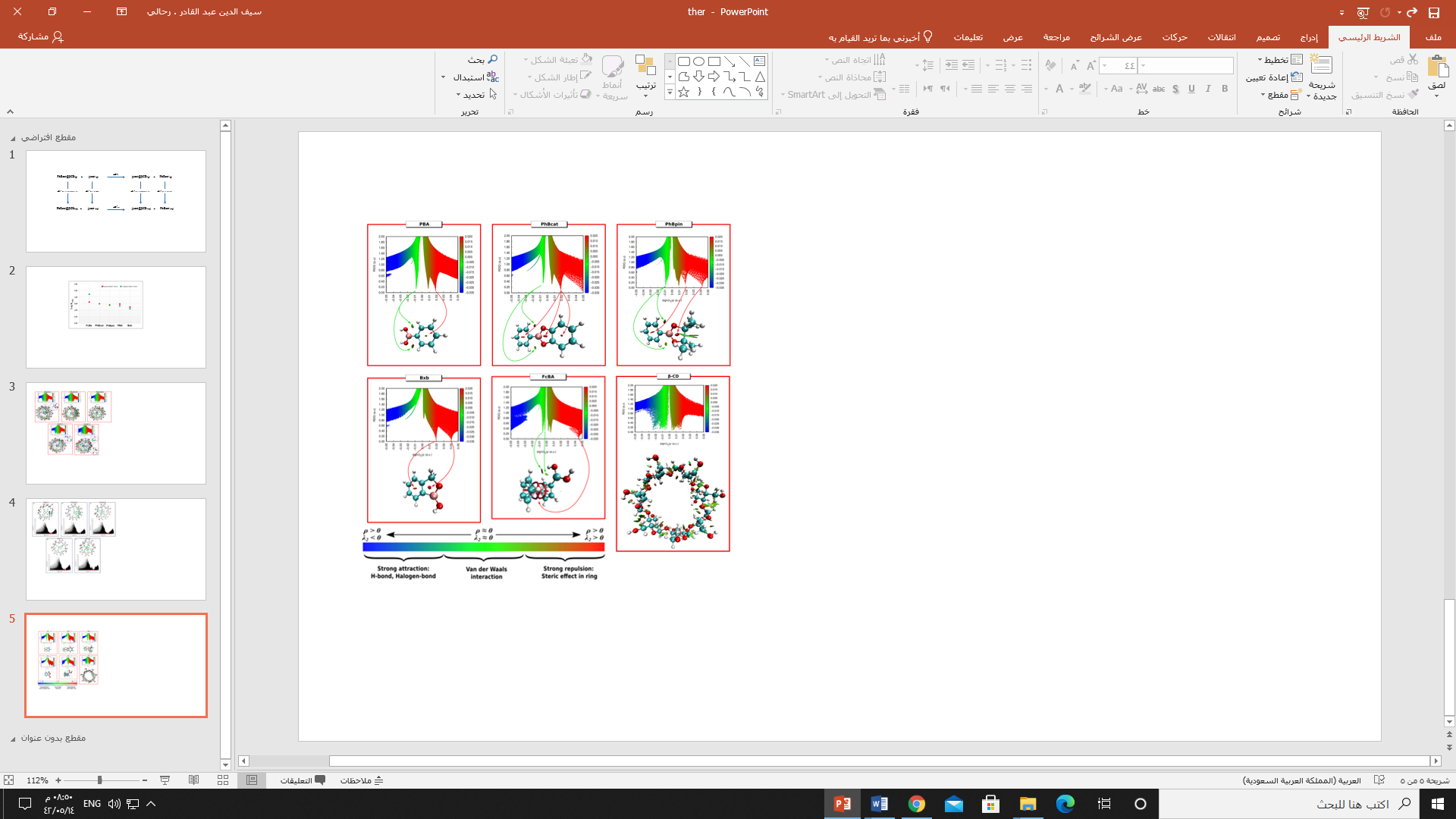


Fig. S1. Calculated thermodynamic parameters for the three most stable conformers of Bxb@β-CD at the BLYP-D3(BJ)/def2-SVP level of theory.

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 3.38451  C -0.02174 0.01350 4.94054  C -0.70370 1.04390 5.64429  C -0.53852 1.21367 7.03341  C 0.31667 0.35147 7.75280  C 1.00299 -0.67958 7.07551  C 0.83388 -0.84365 5.68640  O -1.07036 0.69044 2.72574  O 0.49623 -1.19523 2.76519  H -1.37342 1.72334 5.08911  H -1.07612 2.02177 7.56043  H 0.44936 0.48475 8.84143  H 1.67225 -1.35752 7.63455  H 1.37458 -1.65276 5.16568  H -1.16772 0.53914 1.76389  H 0.35373 -1.28382 1.80111 | B -0.20931 -0.17453 3.37641  C -0.02050 0.01463 4.93930  C -0.70320 1.04380 5.64647  C -0.53970 1.21361 7.03720  C 0.31668 0.35151 7.75770  C 1.00490 -0.67862 7.07874  C 0.83568 -0.84121 5.68791  O -1.06332 0.69237 2.71795  O 0.48822 -1.19843 2.76025  H -1.37484 1.72573 5.09585  H -1.07909 2.02052 7.56414  H 0.44800 0.48398 8.84647  H 1.67491 -1.35672 7.63662  H 1.38004 -1.65134 5.17179  H -1.15451 0.52592 1.75444  H 0.33482 -1.27622 1.79337 |
| **PhBcat** | C 0.75596 -0.42178 7.07404  C -0.08456 0.71471 7.14193  C -0.24111 -0.06482 3.49021  C 0.38754 -1.07390 2.70785  C -1.11139 0.84997 2.83292  C -1.34712 0.75753 1.44804  C -0.71486 -0.25220 0.69019  C 0.15507 -1.16715 1.32222  B 0.00807 0.02893 5.01854  O -0.55498 1.00539 5.86639  O 0.82282 -0.85590 5.75502  C 1.37489 -0.95374 8.21149  C 1.11928 -0.29483 9.44058  C -0.34207 1.37333 8.35034  C 0.28029 0.84257 9.50819  H 1.06590 -1.79484 3.19686  H -1.60950 1.64147 3.41930  H -2.02723 1.47362 0.95402  H -0.90285 -0.32750 -0.39557  H 0.65097 -1.95681 0.73095  H 2.02393 -1.84214 8.14796  H 1.58497 -0.67967 10.36341  H -0.99580 2.25953 8.39243  H 0.10456 1.32851 10.48278 | C 0.75400 -0.42301 7.07807  C -0.08156 0.71608 7.14489  C -0.24130 -0.06524 3.48930  C 0.39144 -1.07202 2.70507  C -1.11598 0.84740 2.83221  C -1.35200 0.75512 1.44637  C -0.71543 -0.25224 0.68691  C 0.15895 -1.16502 1.31841  B 0.00803 0.02859 5.01792  O -0.55135 1.00791 5.86613  O 0.81936 -0.85891 5.75639  C 1.37163 -0.95843 8.21501  C 1.11778 -0.29658 9.44424  C -0.33809 1.37837 8.35190  C 0.28269 0.84507 9.51086  H 1.07397 -1.79294 3.18861  H -1.61947 1.63819 3.41521  H -2.03511 1.46898 0.95357  H -0.90309 -0.32703 -0.39880  H 0.65821 -1.95208 0.72676  H 2.01746 -1.84953 8.15417  H 1.58208 -0.68300 10.36710  H -0.98794 2.26752 8.39510  H 0.10852 1.33308 10.48469 |
| **PhBpin** | C 0.21840 0.15725 -1.49224  C 1.50734 0.47346 -2.00257  C 1.72080 0.64417 -3.38454  C 0.64591 0.49654 -4.28750  C -0.64130 0.17877 -3.80244  C -0.85028 0.01364 -2.41912  B -0.01846 -0.02208 0.04494  O -1.25108 -0.34159 0.59334  C -1.14128 -0.21329 2.05774  C -1.96739 -1.33884 2.71394  C -1.73733 1.16727 2.43567  O 0.98304 0.12638 0.99219  C 0.44472 -0.31216 2.29255  C 0.99854 0.61674 3.39265  C 0.94567 -1.76112 2.52343  H 2.35184 0.58936 -1.30098  H 2.72748 0.89537 -3.76266  H 0.81191 0.63173 -5.37122  H -1.48382 0.06145 -4.50671  H -1.85931 -0.23224 -2.04473  H -1.67594 -2.34097 2.34023  H -1.84595 -1.32569 3.82036  H -3.04727 -1.19628 2.48849  H -2.78058 1.22970 2.05782  H -1.76000 1.31669 3.53686  H -1.16494 2.00410 1.98216  H 0.80174 1.68614 3.17395  H 0.54946 0.37051 4.38036  H 2.09962 0.48710 3.47916  H 2.05604 -1.77638 2.46730  H 0.64642 -2.14391 3.52352  H 0.55920 -2.46202 1.75249 | C 0.21900 0.15777 -1.49601  C 1.50913 0.47111 -2.00878  C 1.72328 0.64165 -3.39183  C 0.64695 0.49687 -4.29540  C -0.64177 0.18219 -3.80917  C -0.85034 0.01729 -2.42448  B -0.01839 -0.02193 0.04410  O -1.24970 -0.34565 0.58950  C -1.14109 -0.21393 2.06491  C -1.96422 -1.33982 2.72082  C -1.73776 1.16658 2.43591  O 0.98263 0.13167 0.98903  C 0.44250 -0.31286 2.29927  C 0.99369 0.61641 3.39833  C 0.94595 -1.76034 2.52340  H 2.35843 0.58609 -1.31243  H 2.73070 0.89022 -3.76920  H 0.81256 0.63149 -5.37906  H -1.48514 0.06724 -4.51261  H -1.86219 -0.22587 -2.05519  H -1.67110 -2.34254 2.34929  H -1.83511 -1.32268 3.82572  H -3.04570 -1.19566 2.50309  H -2.78341 1.22571 2.06322  H -1.75762 1.31469 3.53673  H -1.16608 2.00393 1.98197  H 0.79684 1.68611 3.17990  H 0.53620 0.36884 4.38110  H 2.09356 0.48164 3.49394  H 2.05698 -1.77359 2.47361  H 0.64458 -2.14164 3.52276  H 0.55985 -2.46120 1.75195 |
| **Bxb** | C -0.77268 1.86885 6.28432  C -0.18419 1.33792 7.45287  C -0.64440 1.14754 5.08195  C 0.05853 -0.08703 5.02653  C 0.64097 -0.60430 6.20573  C 0.51815 0.10934 7.41621  H -1.31750 2.82889 6.32223  H -0.27217 1.88641 8.40708  H 1.19053 -1.56391 6.19277  H 0.96950 -0.28765 8.34192  C -1.18157 1.49213 3.69776  O -0.76760 0.42349 2.81603  B -0.04270 -0.53387 3.51809  O 0.43625 -1.63308 2.84736  H -0.77988 2.46263 3.31665  H -2.29658 1.57116 3.68521  H 0.92433 -2.24400 3.43440 | C -0.77462 1.87136 6.28367  C -0.18542 1.33921 7.45252  C -0.64494 1.14843 5.08116  C 0.05929 -0.08662 5.02824  C 0.64325 -0.60655 6.20709  C 0.51865 0.10940 7.41710  H -1.31996 2.83070 6.31888  H -0.27403 1.88762 8.40676  H 1.19165 -1.56577 6.18871  H 0.96962 -0.28555 8.34389  C -1.18365 1.49768 3.70106  O -0.76483 0.42024 2.81495  B -0.03867 -0.53640 3.52618  O 0.43505 -1.63201 2.84642  H -0.78021 2.46528 3.31880  H -2.29749 1.57242 3.68715  H 0.92530 -2.25492 3.42451 |
| **FcBA** | Fe 0.00010 0.00246 5.00003  C 1.06795 -0.33767 3.24157  C -0.27357 -0.89586 3.14026  H -0.50242 -1.95940 2.97663  C -1.23702 0.16182 3.30839  H -2.33220 0.05146 3.29332  C -0.51395 1.39489 3.51688  H -0.95951 2.38737 3.68301  C 0.89551 1.09172 3.47710  H 1.69975 1.83458 3.60594  C 1.24905 -0.25205 6.65002  H 2.34906 -0.22049 6.62082  C 0.43384 -1.43124 6.45030  H 0.80538 -2.44611 6.24337  C -0.95208 -1.03567 6.54718  H -1.82282 -1.69912 6.43531  C -0.99500 0.38609 6.80313  H -1.90374 0.99445 6.92439  C 0.36539 0.87047 6.86805  H 0.67154 1.91199 7.04811  B 2.39776 -1.16202 3.32212  O 3.62445 -0.61225 3.67927  H 3.56770 0.33841 3.90171  O 2.35529 -2.51522 3.04683  H 3.23514 -2.93350 3.16230 | Fe -0.00058 -0.00028 4.99861  C 1.06641 -0.34142 3.24096  C -0.27796 -0.89992 3.14197  H -0.51630 -1.96256 2.98214  C -1.24066 0.16064 3.30885  H -2.33636 0.05160 3.29512  C -0.51405 1.39354 3.51438  H -0.95847 2.38682 3.68133  C 0.89600 1.08968 3.47468  H 1.70530 1.82595 3.60724  C 1.25181 -0.24859 6.64720  H 2.35162 -0.21177 6.61226  C 0.43642 -1.42987 6.45211  H 0.80858 -2.44585 6.24934  C -0.95117 -1.03498 6.54921  H -1.82220 -1.69916 6.43988  C -0.99444 0.38852 6.80215  H -1.90353 0.99703 6.92231  C 0.36695 0.87407 6.86420  H 0.67383 1.91665 7.03813  B 2.40031 -1.16008 3.32279  O 3.61861 -0.60954 3.69954  H 3.56148 0.33656 3.95000  O 2.36573 -2.50849 3.01289  H 3.23827 -2.94347 3.13871 |
| **PBA@β-CD** | C 5.72897 -2.99410 0.23050  C 6.43020 -2.16484 1.33764  C 5.91622 -0.71183 1.35048  C 5.91633 -0.07324 -0.06597  C 5.32491 -1.03255 -1.14495  C 5.54207 -0.55539 -2.58556  C 1.21113 -5.94698 0.50286  C 2.14643 -5.92892 1.73926  C 2.98892 -4.63765 1.78897  C 3.68941 -4.40160 0.42676  C 2.66113 -4.42723 -0.73662  C 3.25461 -4.22858 -2.16050  C -3.96499 -4.59484 -0.03120  C -3.50196 -5.42877 1.19721  C -2.03108 -5.12693 1.55037  C -1.15656 -5.30763 0.28760  C -1.67948 -4.42366 -0.87553  C -0.89127 -4.57356 -2.20761  C -6.43662 0.23176 0.24286  C -6.82573 -0.84556 1.29213  C -5.69878 -1.88845 1.46232  C -5.24426 -2.46297 0.09358  C -4.95818 -1.31026 -0.91721  C -4.67457 -1.80846 -2.34007  C -3.84674 4.86348 1.15088  C -4.55495 4.26037 2.38937  C -4.74224 2.73830 2.23075  C -5.43602 2.41851 0.88537  C -4.74598 3.13207 -0.31542  C -5.50554 2.99196 -1.64374  C 1.39825 5.71147 0.32820  C 0.72787 6.18702 1.64398  C -0.50857 5.32810 1.97278  C -1.45011 5.27311 0.74506  C -0.69334 4.79992 -0.52470  C -1.55967 4.74279 -1.81435  C 5.50855 2.35345 -0.50177  C 5.59277 3.42422 0.62558  C 4.19282 3.79035 1.16020  C 3.26292 4.14442 -0.02345  C 3.22420 2.97799 -1.04622  C 2.30688 3.21881 -2.27450  O 6.22647 -2.81158 2.61009  O 6.73003 0.01876 2.27302  O 5.10076 1.11122 0.06714  O 5.94230 -2.35408 -1.03580  O 4.79307 -1.41642 -3.46014  O 1.35398 -6.10434 2.92961  O 3.91392 -4.78806 2.87104  O 4.34493 -3.11144 0.53186  O 1.97907 -5.73532 -0.69627  H 3.19094 -3.14844 -2.42435  O 4.58765 -4.72043 -2.33080  O -4.38217 -5.18794 2.31434  O -1.66854 -6.01577 2.61267  O 0.20064 -4.95954 0.65500  O -3.08239 -4.79775 -1.13191  O -0.41981 -5.89063 -2.49998  O -7.12512 -0.19780 2.54467  O -6.19702 -2.89525 2.34461  O -4.03655 -3.21499 0.33698  O -6.10393 -0.41326 -0.99658  O -3.93332 -0.78925 -3.09065  O -3.79627 4.59207 3.56878  O -5.50477 2.28985 3.35796  O -5.33558 0.98136 0.73675  O -4.60001 4.56771 -0.03714  O -6.89269 3.32502 -1.45378  O 1.70114 6.16069 2.70469  O -1.13043 5.90799 3.12542  O -2.52303 4.35427 1.06898  O 0.43780 5.71638 -0.74618  O -2.54291 5.77304 -1.95010  O 6.45853 2.94890 1.67869  O 4.36972 4.87492 2.07958  O 1.95256 4.42012 0.52726  O 4.60204 2.77039 -1.51966  O 2.31374 4.54576 -2.80614  H 6.20034 -4.00011 0.14135  H 7.52160 -2.14592 1.08750  H 4.84920 -0.73269 1.68796  H 6.96718 0.20051 -0.33503  H 4.22793 -1.11525 -0.96805  H 6.64041 -0.58188 -2.81463  H 5.19750 0.50516 -2.66015  H 0.75754 -6.95920 0.38478  H 2.85535 -6.78830 1.62036  H 2.29353 -3.77569 1.96591  H 4.44827 -5.19719 0.24275  H 1.89473 -3.63624 -0.56448  H -4.96381 -4.95379 -0.37844  H -3.56306 -6.50700 0.89953  H -1.95232 -4.05563 1.87251  H -1.19638 -6.37147 -0.04593  H -1.64595 -3.34867 -0.58200  H -0.06716 -3.82021 -2.20413  H -1.58605 -4.27282 -3.02680  H -7.29800 0.89686 0.00512  H -7.73512 -1.37445 0.90648  H -4.80868 -1.36438 1.89849  H -6.04894 -3.13185 -0.30531  H -4.06972 -0.74846 -0.54477  H -5.64511 -2.02572 -2.84395  H -4.07607 -2.74671 -2.29789  H -3.83785 5.97673 1.22043  H -5.57140 4.72746 2.44257  H -3.73047 2.25682 2.20940  H -6.50383 2.73190 0.94280  H -3.73908 2.67576 -0.45470  H -5.38311 1.93874 -2.00046  H -5.01103 3.66755 -2.38816  H 2.18594 6.43774 0.01838  H 0.37919 7.23761 1.47017  H -0.16202 4.28449 2.18399  H -1.86588 6.28849 0.54375  H -0.28502 3.77991 -0.34495  H -2.00780 3.72162 -1.86626  H -0.85995 4.82675 -2.67899  H 6.50176 2.24978 -1.00145  H 6.03102 4.34757 0.16701  H 3.75771 2.89305 1.67171  H 3.65037 5.04820 -0.55137  H 2.87150 2.04724 -0.54204  H 1.27778 2.88173 -1.99439  H 2.65559 2.52859 -3.07790  H 6.54761 -2.18043 3.29296  H 6.49014 0.97928 2.20340  H 4.89455 -1.08439 -4.37601  H 1.95206 -5.91200 3.68674  H 4.53657 -4.01736 2.86559  H 5.17145 -3.92727 -2.31269  H -3.92471 -5.56733 3.09972  H -0.71089 -5.87748 2.82553  H 0.46994 -5.97939 -2.08163  H -7.21771 -0.92499 3.20236  H -5.50159 -3.59619 2.45318  H -4.22277 -0.81629 -4.02644  H -4.16616 4.04527 4.29789  H -5.84349 1.37942 3.16456  H -7.33131 3.29221 -2.32902  H 1.19411 6.28230 3.53940  H -1.91314 5.35307 3.37425  H -3.34100 5.48631 -1.44565  H 6.34419 3.58746 2.41995  H 3.47880 5.15149 2.41400  H 1.65911 5.07328 -2.28848  H 2.57713 -4.77089 -2.86420  B -1.19993 0.03903 -1.32169  C -0.12251 0.21155 -0.18255  C -0.25950 1.20669 0.82417  C 0.67906 1.32131 1.87035  C 1.76921 0.42917 1.94201  C 1.91963 -0.57512 0.96117  C 0.98751 -0.67245 -0.09058  O -2.19726 0.99926 -1.45451  O -1.14128 -1.08210 -2.13352  H -1.12155 1.89422 0.79565  H 0.55556 2.10320 2.63991  H 2.50010 0.51010 2.76621  H 2.75400 -1.29081 1.02220  H 1.11434 -1.45811 -0.85574  H -2.89382 0.73016 -2.09866  H -1.90977 -1.13208 -2.75060 | C 5.46525 -2.91933 -0.44535  C 6.33032 -2.17583 0.61111  C 5.78713 -0.75502 0.87603  C 5.54441 0.01932 -0.44720  C 4.70490 -0.83583 -1.44008  C 4.54411 -0.21011 -2.82946  C 1.26187 -6.17261 0.39315  C 2.30239 -6.10748 1.54761  C 3.06076 -4.76626 1.50018  C 3.65556 -4.52993 0.09149  C 2.58793 -4.70111 -1.02849  C 3.15486 -4.64452 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2.67958  C 2.01081 -0.92487 2.02496  C 1.17521 -1.11515 0.90506  O -1.49862 0.72133 -1.16377  O -0.60549 -1.51965 -1.47348  H -0.23457 2.01357 0.72703  H 1.25299 2.36535 2.70931  H 2.69351 0.47767 3.55529  H 2.64418 -1.75182 2.38695  H 1.14840 -2.09858 0.40882  H -2.11811 0.44910 -1.88334  H -1.31747 -1.56550 -2.16229 |
| **PhBcat@β-CD** | C 2.77726 -5.73358 -0.71415  C 3.79592 -5.57756 0.44441  C 4.19017 -4.09939 0.64315  C 4.63995 -3.45375 -0.69583  C 3.60317 -3.73502 -1.82514  C 4.05072 -3.26526 -3.21375  C -2.60725 -5.74809 -0.48170  C -1.81140 -6.45810 0.64327  C -0.40570 -5.84293 0.80222  C 0.30746 -5.79723 -0.57220  C -0.56276 -5.07567 -1.63644  C 0.05015 -5.03578 -3.06610  C -6.12807 -1.69822 -0.23683  C -6.20096 -2.83481 0.82266  C -4.81921 -3.48706 1.02975  C -4.22804 -3.90102 -0.33836  C -4.19065 -2.69502 -1.31415  C -3.64139 -3.02357 -2.73163  C -5.18157 3.52984 0.83007  C -5.86339 2.71369 1.95845  C -5.57875 1.20611 1.80656  C -5.90593 0.71255 0.37202  C -5.25791 1.63957 -0.70109  C -5.67096 1.32144 -2.14278  C -0.36154 5.93907 0.85731  C -1.19484 5.91461 2.16368  C -2.12224 4.68425 2.19000  C -2.98362 4.66153 0.90566  C -2.07510 4.69493 -0.35658  C -2.83366 4.69599 -1.71461  C 4.53225 3.83218 0.05634  C 4.25098 4.56587 1.39449  C 2.74724 4.55086 1.72650  C 1.91973 5.04219 0.51482  C 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5.41815 1.92220 2.40600  H 4.72040 3.50324 -2.27988  H -0.84552 -5.28528 -3.76900  C 1.70980 0.96733 2.90342  C 0.51292 1.70599 3.05600  C -0.04322 0.16451 -0.30385  C 0.74166 -0.71728 -1.10038  C -1.25330 0.67160 -0.85928  C -1.66073 0.32164 -2.16302  C -0.85792 -0.54555 -2.93787  C 0.34289 -1.06811 -2.40668  B 0.42594 0.61338 1.10539  O -0.30082 1.48035 1.94896  O 1.65631 0.26516 1.70047  C 2.74345 1.02850 3.84569  C 2.52701 1.87093 4.96686  C 0.28623 2.53699 4.16062  C 1.32731 2.60650 5.12078  H 1.68059 -1.12893 -0.69260  H -1.87450 1.35846 -0.25845  H -2.59503 0.73277 -2.58262  H -1.16708 -0.81281 -3.96295  H 0.97394 -1.73664 -3.01767  H 3.68667 0.47613 3.71358  H 3.31632 1.95472 5.73385  H -0.64573 3.11362 4.27291  H 1.19811 3.25400 6.00444 |
| **PhBpin@β-CD** | C -6.34574 -1.21099 -0.57528  C -6.48692 -2.46107 0.33117  C -5.18806 -3.29265 0.32234  C -4.69290 -3.57130 -1.12281  C -4.67894 -2.27271 -1.98478  C -4.34209 -2.49499 -3.47714  C -4.51066 3.74689 0.45671  C -5.29461 3.04763 1.59635  C -5.20265 1.51339 1.46790  C -5.61176 1.07815 0.03797  C -4.78757 1.83206 -1.03950  C -5.17055 1.51862 -2.51063  C 0.41558 5.80171 0.09094  C -0.51617 6.18224 1.28110  C -1.50555 5.04146 1.60701  C -2.22787 4.60843 0.30829  C -1.18635 4.19765 -0.76353  C -1.76608 3.68269 -2.10029  C 5.30594 3.51580 0.39004  C 4.91257 4.45231 1.56147  C 3.38131 4.58635 1.67343  C 2.73648 4.92692 0.30255  C 3.24040 3.96051 -0.81172  C 2.75729 4.29378 -2.24177  C 6.10135 -1.79892 0.28628  C 6.48236 -1.08678 1.60885  C 5.68721 0.22470 1.76444  C 5.80944 1.09263 0.48736  C 5.45315 0.28602 -0.79133  C 5.61618 1.04839 -2.13719  C 2.35844 -5.49881 -0.82333  C 3.18889 -5.64748 0.47838  C 3.68087 -4.27650 0.98633  C 4.39111 -3.51848 -0.16457  C 3.45970 -3.39948 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3.19167 2.10824  H 2.86989 6.09704 1.08332  H 2.50040 3.45008 -0.50618  H 3.17894 6.26873 -1.56474  H 1.50776 5.59914 -1.51815  H 6.52176 -2.30289 -1.45747  H 7.44016 -0.65994 0.13110  H 4.58666 -0.37086 1.28760  H 6.29874 1.60812 -0.37407  H 3.72492 0.05454 -1.13309  H 3.46027 1.96437 -2.43913  H 4.47845 0.92995 -3.47631  H 2.19276 -6.80317 -1.78512  H 4.29141 -6.39005 -0.53595  H 2.93944 -3.82195 0.53466  H 5.37236 -4.09958 -1.34637  H 2.51132 -3.12539 -2.03873  H 4.14884 -2.06425 -3.45458  H 3.26690 -3.32525 -4.39914  H -3.96351 -5.96834 -1.27988  H -2.18020 -7.26216 -0.17408  H -0.82351 -4.55430 0.44734  H 0.10770 -6.87066 -1.37782  H -0.90587 -4.06010 -2.19847  H 0.67654 -4.88666 -3.80617  H -0.98571 -5.01334 -4.49276  H -6.41870 -2.31130 2.30423  H -4.35227 -4.66727 1.42183  H -2.80663 -1.25331 -3.93852  H -5.84811 3.52745 3.02896  H -6.19491 0.35350 1.97535  H -5.47631 0.22349 -3.09645  H -0.50356 5.73728 4.30918  H -3.43721 4.59494 3.02604  H -3.34664 7.04337 -2.40118  H 4.72280 3.38359 3.88877  H 1.84178 5.01652 3.50515  H 2.65426 5.13290 -3.56481  H 6.83889 -1.80639 2.16778  H 5.74991 1.30963 2.50693  H 5.10958 3.34847 -2.19490  H 3.31460 -6.37366 1.67302  H 5.24800 -3.63030 1.34781  H 5.69441 -3.30870 -4.60008  H -2.41623 -6.24599 2.02910  H 0.82962 -6.22003 1.19533  H 0.43936 -6.97194 -4.72910  H -3.65746 2.37637 -3.22212  C -0.40695 0.14670 -1.19931  C -1.11716 -0.85560 -0.48535  C -1.40195 -0.70760 0.88784  C -0.98224 0.45158 1.57692  C -0.26201 1.45402 0.89031  C 0.02301 1.29807 -0.48052  B -0.10499 0.06170 -2.73322  O 1.01856 0.63963 -3.28734  C 0.83537 0.68351 -4.75732  C 2.19300 0.44458 -5.44530  C 0.31061 2.10506 -5.08255  O -0.94400 -0.52848 -3.67860  C -0.23599 -0.47904 -4.99973  C -1.26034 -0.18189 -6.11109  C 0.39200 -1.87705 -5.20546  H -1.44407 -1.77402 -1.00032  H -1.95385 -1.49957 1.42267  H -1.21233 0.57206 2.64989  H 0.07743 2.36139 1.41720  H 0.58159 2.08711 -1.01361  H 2.70310 -0.45846 -5.05332  H 2.05537 0.32301 -6.54190  H 2.86213 1.31606 -5.28231  H 1.00808 2.85056 -4.64281  H 0.25223 2.27776 -6.17842  H -0.69590 2.28758 -4.64774  H -1.84178 0.74099 -5.91124  H -0.73729 -0.06065 -7.08460  H -1.97767 -1.02413 -6.21248  H -0.40871 -2.64707 -5.17205  H 0.89525 -1.95322 -6.19255  H 1.13457 -2.11865 -4.41595 |
| **Bxb@β-CD** | C -0.33534 6.40493 -2.38806  C -1.32056 6.75691 -1.24423  C -2.34014 5.62032 -1.02218  C -3.01085 5.18040 -2.35193  C -1.95587 4.96686 -3.48126  C -2.56871 4.72374 -4.86534  C 4.40576 3.84707 -2.09220  C 4.03327 4.82451 -0.94786  C 2.50356 4.96417 -0.81664  C 1.88659 5.32079 -2.19114  C 2.33095 4.31948 -3.29262  C 1.82794 4.66008 -4.72666  C 5.57324 -1.39122 -1.87614  C 6.22501 -0.38914 -0.88144  C 5.30413 0.82295 -0.64007  C 4.91708 1.44279 -2.00289  C 4.28060 0.38629 -2.94547  C 3.95711 0.92512 -4.37115  C 2.52136 -5.64153 -0.41015  C 3.70160 -5.24842 0.52056  C 4.10042 -3.76710 0.33519  C 4.32517 -3.42514 -1.16253  C 3.12686 -3.91654 -2.01757  C 3.32782 -3.79514 -3.53561  C -2.70840 -5.28881 0.83561  C -1.75341 -5.37552 2.05118  C -0.33442 -4.90614 1.67149  C 0.16711 -5.64607 0.40574  C -0.88713 -5.64495 -0.74336  C -0.51640 -6.54414 -1.93339  C -5.95809 -1.29763 -0.70327  C -5.98021 -1.82140 0.75799  C -4.61229 -2.41379 1.15068  C -4.19010 -3.46576 0.09673  C 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-5.05925 2.52311  H 0.02665 -8.41400 -2.24443  H -6.19431 -1.07486 2.55156  H -3.88217 -3.33892 2.74832  H -3.67548 -5.67830 -1.69748  H -6.31679 4.36495 0.45370  H -6.38969 1.15628 1.00146  H -5.78230 -1.27193 -3.40320  H 2.58461 4.25047 -5.43804  C -0.96622 0.85458 -1.99350  C -1.09839 -0.07900 -0.94161  C -0.44168 0.41133 -3.22403  C -0.02395 -0.93437 -3.41597  C -0.16729 -1.85564 -2.35275  C -0.70812 -1.42812 -1.12000  H -1.27139 1.90500 -1.84685  H -1.51810 0.24584 0.02602  H 0.14272 -2.90606 -2.48278  H -0.83548 -2.14334 -0.29074  C -0.21325 1.20362 -4.50367  O 0.35253 0.28639 -5.46230  B 0.52141 -0.98424 -4.90272  O 1.09667 -1.96571 -5.64988  H 0.49625 2.05030 -4.34490  H -1.14644 1.65539 -4.91564  H 1.27959 -2.81157 -5.16913 | C -0.39643 6.27464 -2.44602  C -1.31883 6.66307 -1.25891  C -2.33111 5.53649 -0.95726  C -3.07962 5.09087 -2.24306  C -2.09081 4.83068 -3.42001  C -2.79193 4.59989 -4.76383  C 4.39196 3.79726 -2.09262  C 3.93747 4.62471 -0.85649  C 2.39927 4.73694 -0.79221  C 1.85001 5.25616 -2.14420  C 2.39527 4.41879 -3.33703  C 1.98930 4.94666 -4.72150  C 5.67431 -1.44071 -1.93767  C 6.34436 -0.39298 -1.00693  C 5.42376 0.82691 -0.79228  C 4.97588 1.39937 -2.16518  C 4.35720 0.28572 -3.05968  C 4.00536 0.73866 -4.48403  C 2.62069 -5.60971 -0.30832  C 3.81723 -5.20777 0.59956  C 4.22760 -3.73681 0.36146  C 4.42147 -3.44089 -1.15142  C 3.20179 -3.94199 -1.97317  C 3.37527 -3.83283 -3.49598  C -2.61680 -5.22202 0.88437  C -1.67383 -5.27917 2.11291  C -0.24887 -4.81526 1.74174  C 0.25986 -5.56231 0.48129  C -0.77175 -5.54326 -0.68411  C -0.39006 -6.41340 -1.89044  C -6.00880 -1.41505 -0.78446  C -6.06872 -1.95587 0.67556  C -4.68177 -2.45773 1.12923  C -4.14362 -3.47063 0.09013  C -4.12687 -2.85705 -1.33499  C -3.64159 -3.82445 -2.44606  C -5.17946 3.74760 -2.17803  C -5.95560 3.46549 -0.86245  C -5.58317 2.08545 -0.28152  C -5.75200 0.98884 -1.36318  C -5.01084 1.36596 -2.67988  C -5.26841 0.39377 -3.84012  O -0.49698 6.96707 -0.11118  O -3.22510 6.02685 0.05004  O -3.78257 3.87000 -1.89695  O -1.19969 5.97452 -3.58922  O -1.83002 4.10586 -5.71552  O 4.48552 4.02936 0.33760  O 2.07659 5.61332 0.29746  O 0.40874 5.15576 -2.07022  O 3.85394 4.37726 -3.28455  H 0.89043 4.79786 -4.84917  O 2.35118 6.33526 -4.84534  O 6.70374 -1.02722 0.23859  O 6.16547 1.77707 -0.01211  O 3.98617 2.43452 -1.93902  O 5.30396 -0.82672 -3.17613  O 5.14699 1.34051 -5.11363  O 3.44727 -5.44646 1.97498  O 5.42139 -3.49392 1.11751  O 4.54131 -2.00214 -1.27599  O 2.94827 -5.34887 -1.67697  O 2.11907 -3.99447 -4.19735  O -2.26573 -4.47708 3.15388  O 0.60480 -5.04904 2.87134  O 1.46671 -4.86910 0.08518  O -2.08174 -6.00041 -0.20377  O -0.10298 -7.75580 -1.46443  O -6.58820 -0.92681 1.54316  O -4.83454 -3.04920 2.43158  O -2.80908 -3.86428 0.50287  O -5.48976 -2.42488 -1.65797  O -4.11132 -5.17944 -2.33866  O -5.70159 4.53459 0.07464  O -6.42640 1.86515 0.85715  O -5.20364 -0.23573 -0.81586  O -5.42754 2.70114 -3.11820  O -6.68088 0.25683 -4.07544  H 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0.67061  H -3.98038 -1.58571 1.16916  H -4.81117 -4.36409 0.07258  H -3.45355 -1.96781 -1.35318  H -2.52659 -3.77824 -2.48203  H -4.00780 -3.42149 -3.41835  H -5.56343 4.67949 -2.65455  H -7.04381 3.44787 -1.12278  H -4.50234 2.10658 0.01649  H -6.83681 0.85822 -1.58292  H -3.91206 1.36571 -2.48395  H -4.80019 -0.58325 -3.57386  H -4.73402 0.78305 -4.74521  H -1.10471 7.08067 0.65545  H -3.96757 5.37384 0.15925  H -2.31841 3.86557 -6.53278  H 4.09859 4.49651 1.11224  H 1.11995 5.87288 0.22018  H 1.90720 6.67987 -5.64989  H 6.93151 -0.30251 0.86674  H 5.54668 2.50773 0.25538  H 4.83593 1.76178 -5.94332  H 4.15935 -5.05713 2.53310  H 5.72622 -2.56754 0.92182  H 1.87691 -4.94571 -4.23186  H -1.67976 -4.52624 3.94186  H 1.54603 -4.95387 2.56776  H 0.29933 -8.22474 -2.22701  H -6.45331 -1.23761 2.46832  H -3.93863 -3.33511 2.74398  H -3.52679 -5.64303 -1.69024  H -6.07097 4.24611 0.94132  H -6.29644 0.92884 1.16778  H -6.81299 -0.57145 -4.58418  H 2.50774 4.31508 -5.48862  C -1.09423 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| **FcBA@β-CD** | C 4.15375 4.72185 0.11145  C 3.62114 5.66432 1.21844  C 2.11157 5.44061 1.46059  C 1.29854 5.48218 0.13300  C 1.98226 4.60647 -0.96640  C 1.37609 4.81247 -2.35690  C 6.19383 -0.18486 0.94460  C 6.13263 0.72465 2.19513  C 5.04035 1.80062 2.04064  C 5.22616 2.56130 0.70667  C 5.38323 1.59650 -0.50794  C 5.72463 2.30831 -1.82582  C 3.69309 -4.85665 0.00031  C 4.32723 -4.58620 1.39519  C 4.35350 -3.07727 1.70949  C 5.05709 -2.33576 0.55209  C 4.39597 -2.66420 -0.81168  C 5.12290 -2.01814 -2.02951  C -1.52948 -6.07609 -0.78063  C -0.76539 -6.70753 0.40939  C 0.43139 -5.83035 0.82809  C 1.32670 -5.50995 -0.39942  C 0.48471 -4.94694 -1.58623  C 1.30405 -4.78953 -2.88621  C -5.69376 -2.65421 -0.52951  C -5.65076 -3.81387 0.50612  C -4.20472 -4.30445 0.71987  C -3.54087 -4.63714 -0.63452  C -3.69318 -3.47836 -1.65160  C -3.18339 -3.82185 -3.08883  C -5.39528 2.55703 0.94666  C -5.69776 1.54323 2.07747  C -5.20257 0.12223 1.73433  C -5.71010 -0.30739 0.33647  C -5.42505 0.79210 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