Supporting Material

Study of *Thermomyces lanuginosa* lipase in presence of tributyrylglycerol and water

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Figure S1: GROMOS topology file of a TBG molecule.

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[ moleculetype ]
; Name            nrexcl
TBG                  3

[ atoms ]
;   nr       type  resnr residue  atom  cgnr      charge        mass  typeB    chargeB       massB
     1        CH3      1    TBG    CA4     1           0      14.027
     2        CH2      1    TBG    CA3     1           0      14.027
     3        CH2      1    TBG    CA2     1           0      14.027
     4          C      1    TBG    CA1     1        0.54      12.011
     5          O      1    TBG    OA1     1       -0.38     15.9994
     6         OA      1    TBG    OG1     1       -0.36     15.9994
     7        CH2      1    TBG    CG1     1         0.2      14.027
     8        CH1      1    TBG    CG2     2         0.2      13.019
     9         OA      1    TBG    OG2     2       -0.36     15.9994
    10          C      1    TBG    CB1     2        0.54      12.011
    11          O      1    TBG    OB1     2       -0.38     15.9994
    12        CH2      1    TBG    CB2     2           0      14.027
    13        CH2      1    TBG    CB3     2           0      14.027
    14        CH3      1    TBG    CB4     2           0      14.027
    15        CH2      1    TBG    CG3     3         0.2      14.027
    16         OA      1    TBG    OG3     3       -0.36     15.9994
    17          C      1    TBG    CC1     3        0.54      12.011
    18          O      1    TBG    OC1     3       -0.38     15.9994
    19        CH2      1    TBG    CC2     3           0      14.027
    20        CH2      1    TBG    CC3     3           0      14.027
    21        CH3      1    TBG    CC4     3           0      14.027   ; qtot 0

[ bonds ]
;  ai   aj funct          c0            c1            c2            c3
    1    2          gb_26
    2    3          gb_26
    3    4          gb_26
    4    5          gb_4
    4    6          gb_12
    6    7          gb_17
    7    8          gb_26
    8    9          gb_17
    8   15          gb_26
    9   10          gb_12
   10   11          gb_4
   10   12          gb_26
   12   13          gb_26
   13   14          gb_26
   15   16          gb_17
   16   17          gb_12
   17   18          gb_4
   17   19          gb_26
   19   20          gb_26
   20   21          gb_26

[ pairs ]
;  ai   aj funct          c0            c1            c2            c3
    1    4
    2    5
    2    6
    3    7
    4    8
    5    7
    6    9
    6   15
    7   10
    7   16
    8   11
    8   12
    8   17
    9   13
    9   16
   10   14
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    10     15
    11     13
    15     18
    15     19
    16     20
    17     21
    18     20

[ angles ]
;  ai    aj    ak funct            c0              c1              c2              c3
    1     2     3              ga_12
    2     3     4              ga_12
    3     4     5              ga_29
    3     4     6              ga_18
    5     4     6              ga_32
    4     6     7              ga_9
    6     7     8              ga_12
    7     8     9              ga_12
    7     8    15              ga_12
    9     8    15              ga_12
    8     9    10              ga_9
    9    10    11              ga_32
    9    10    12              ga_18
   11    10    12              ga_29
   10    12    13              ga_12
   12    13    14              ga_12
    8    15    16              ga_12
   15    16    17              ga_9
   16    17    18              ga_32
   16    17    19              ga_18
   18    17    19              ga_29
   17    19    20              ga_12
   19    20    21              ga_12

[ dihedrals ]
;  ai    aj    ak    al funct            c0              c1              c2              c3
c4          c5
    1     2     3     4              gd_17
    2     3     4     6              gd_20
    3     4     6     7              gd_12
    4     6     7     8              gd_12
    6     7     8    15              gd_17
    7     8     9    10              gd_12
    7     8    15    16              gd_17
    8     9    10    12              gd_12
    9    10    12    13              gd_20
   10    12    13    14              gd_17
    8    15    16    17              gd_12
   15    16    17    19              gd_12
   16    17    19    20              gd_20
   17    19    20    21              gd_17

[ dihedrals ]
;  ai    aj    ak    al funct            c0              c1              c2              c3
    3     5     6     4              gi_1
   10     9    11    12              gi_1
   17    16    18    19              gi_1
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Figure S2: DSSP diagram for different runs and 3 representative snapshots of the secondary TBG-binding pocket. Snapshot panels: the TBG molecule is in orange, the lid fragment in magenta, and the catalytic triad in blue. The secondary TBG-binding pocket is represented by a green surface and the water molecule between the lid and the TBG molecule is shown in red.