Indian Journal of Biochemistry & Biophysics
Vol. 62, April 2025, pp. 426-430
DOI: 10.56042/ijbb.v62i4.14428

Bisphenol B: An inhibitor of mitochondrial electron transport chain protein

Shivani Gupta, Dastagiri Pinjari, Deepak Yadav, Deepak Kumar, Rajasri Bhattacharyya & Dibyajyoti Banerjee*
Department of Experimental Medicine and Biotechnology, Postgraduate Institute of Medical Education and Research, Chandigarh

Received 16 October 2024; revised 05 November 2024

Supplementary Figures

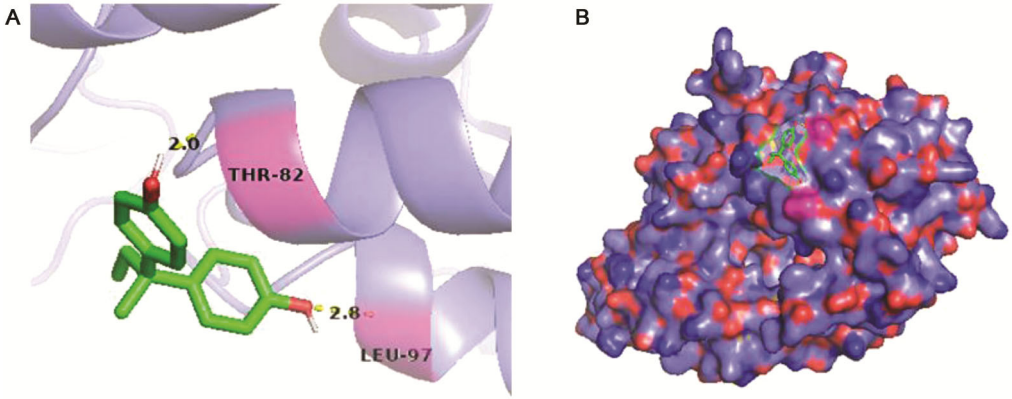

Fig. S1 — Shows the docked complex of NADH dehydrogenase protein (grid centre, Arg88), bonded with Bisphenol B (BPB, in stick mode), in cartoon (A) and surface (B) view. The BPB interacts with Thr-82 and Leu-97. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

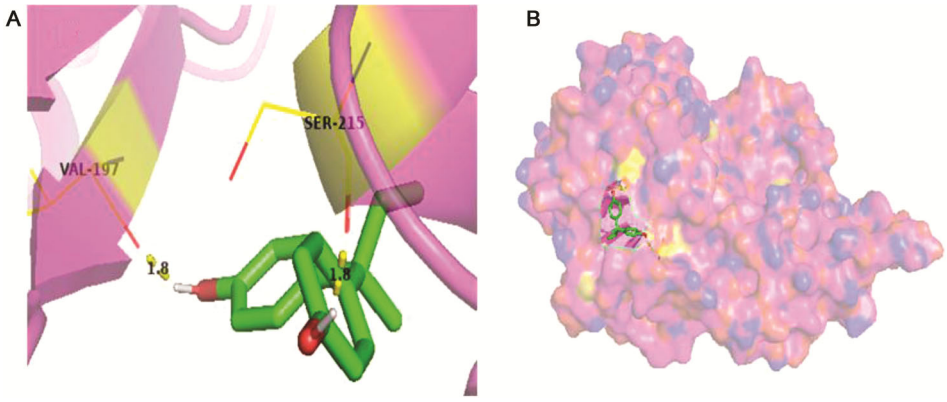

Fig. S2 — Shows the docked complex of NADH dehydrogenase protein (grid centre, Arg199), bonded with Bisphenol B (BPB, in stick mode) in cartoon (A) and surface (B) view. BPB interacts with Val-197 and Ser-215. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

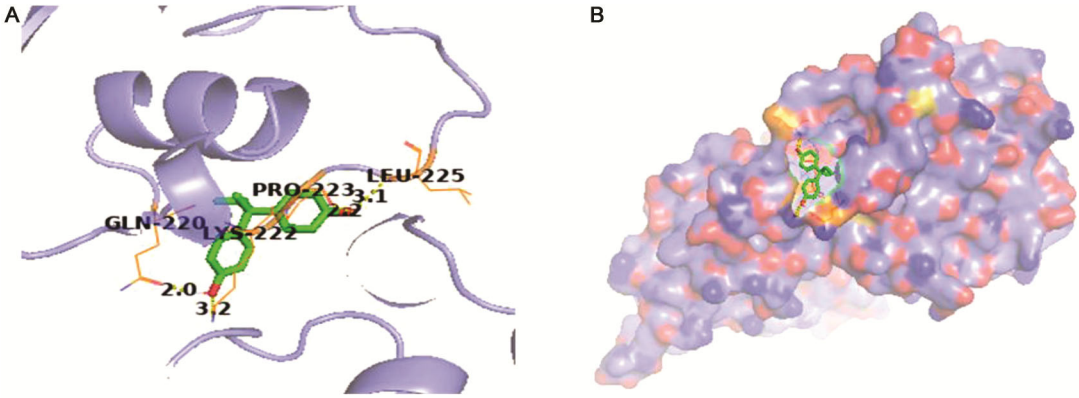

Fig. S3 — Shows the docked complex of NADH dehydrogenase protein (grid centre, Arg224), bonded with Bisphenol B (BPB, in stick mode) in cartoon (A) and surface (B) view. BPB interacts with Gln-220, Lys-222, Pro-223 and Leu-225. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

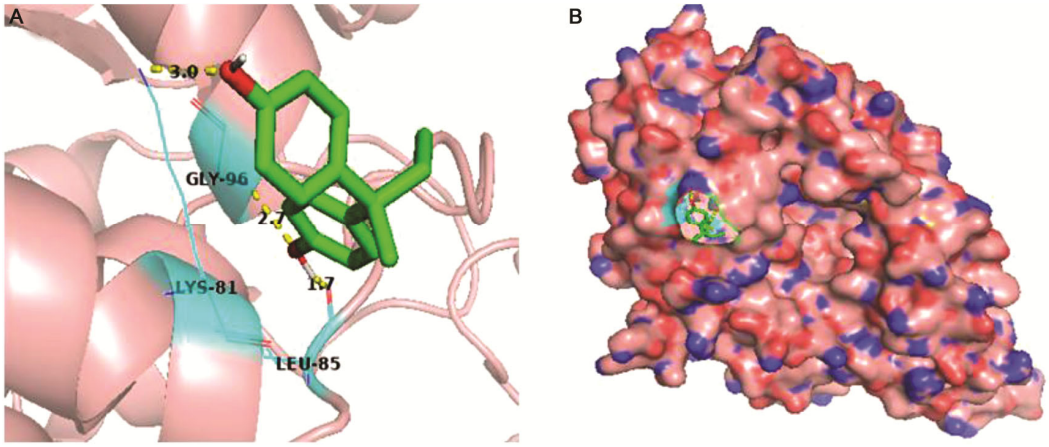

Fig. S4 — Shows the docked complex of NADH dehydrogenase protein (grid centre, Phe93), bonded with Bisphenol B (BPB, in stick mode) in cartoon (A) and surface (B) view. BPB interacts with Lys-81, Leu-85 and Gly-96. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

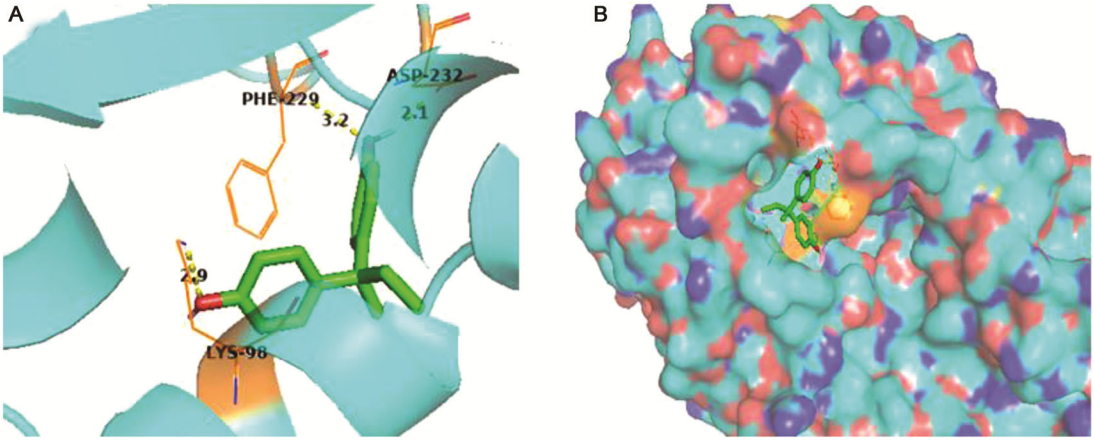

Fig. S5 — Shows the docked complex of NADH dehydrogenase protein (grid centre, Phe 229), bonded with Bisphenol B (BPB, in stick mode) in cartoon (A) and surface (B) view. BPB interacts with Lys-96, Phe-229 and Asp-232. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

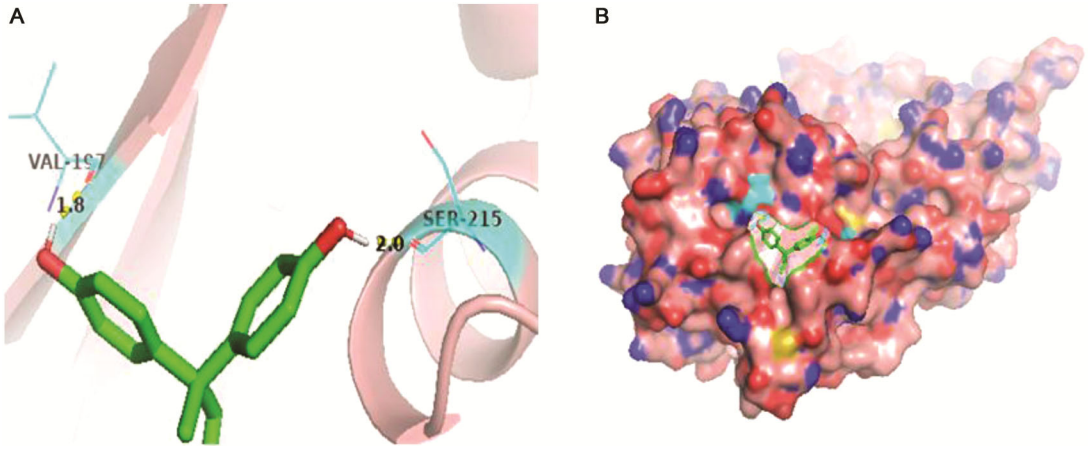

Fig. S6 — Shows the docked complex of NADH dehydrogenase protein (grid centre, Phe 236), bonded with Bisphenol B (BPB, in stick mode) in cartoon (A) and surface (B) view. BPB interacts with Val-197 and Ser-215. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

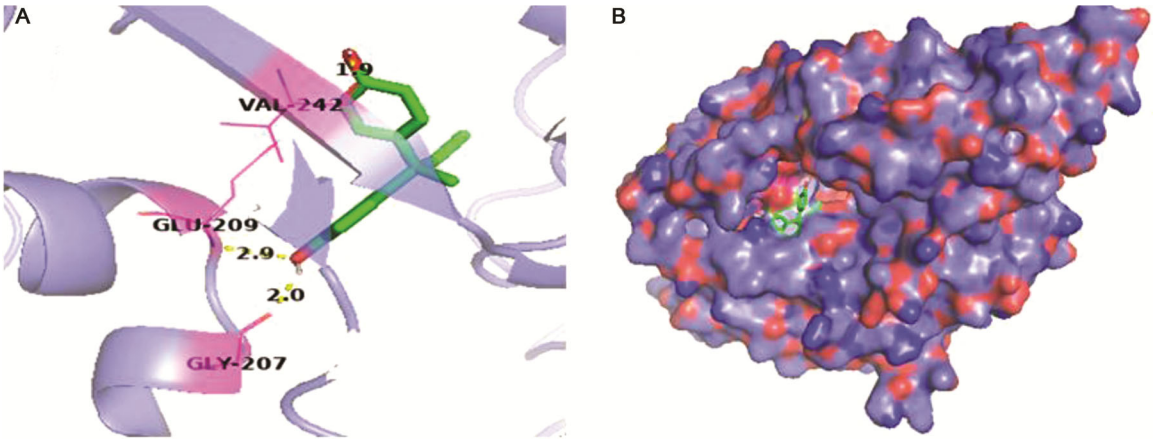

Fig. S7 — Shows the docked complex of NADH Dehydrogenase protein (grid centre, Thr 95), bonded with Bisphenol B (BPB, in stick mode) in cartoon (A) and surface (B) view. BPB interacts with Gly-207, Glu-209 and Val-242. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labeled along with the residue involved.

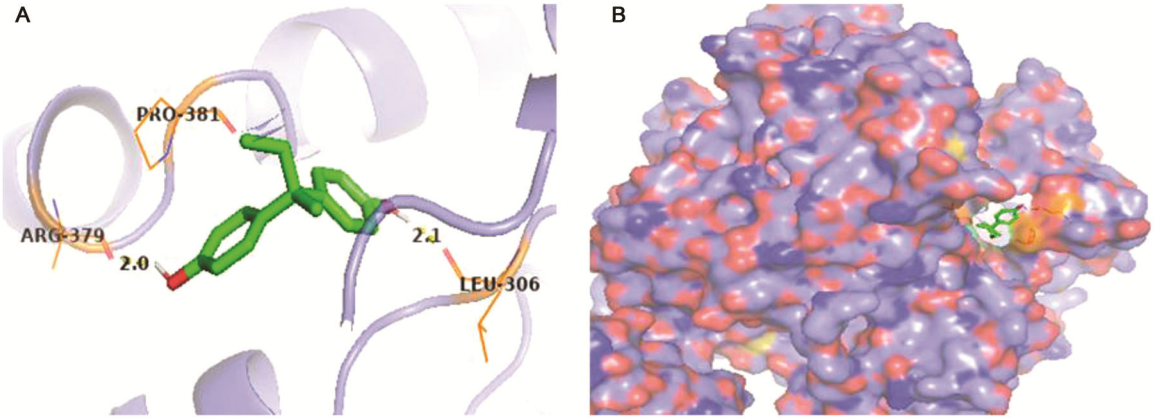

Fig. S8 — Shows the docked complex of Succinate Dehydrogenase protein (grid centre, Arg 340), bonded with Bisphenol B (BPB, in stick mode) in cartoon (A) and surface (B) view. BPB interacts with Arg-379, Pro-381 and Leu-306. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

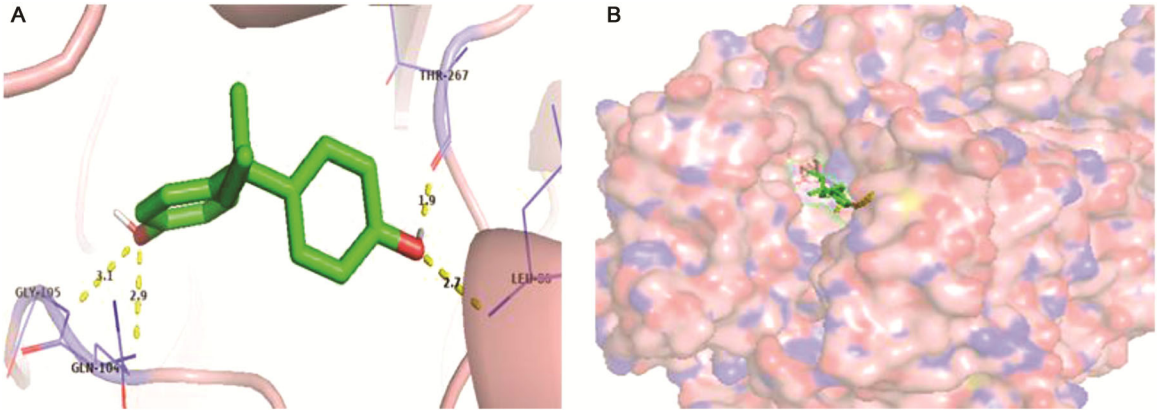

Fig. S9 — Shows the docked complex of Succinate Dehydrogenase protein (grid centre, Arg 451), bonded with Bisphenol B (BPB, in stick mode) in cartoon (A) and surface (B) view. BPB interacts with Gly-104, Gly-105, Thr-267, and Leu-80. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

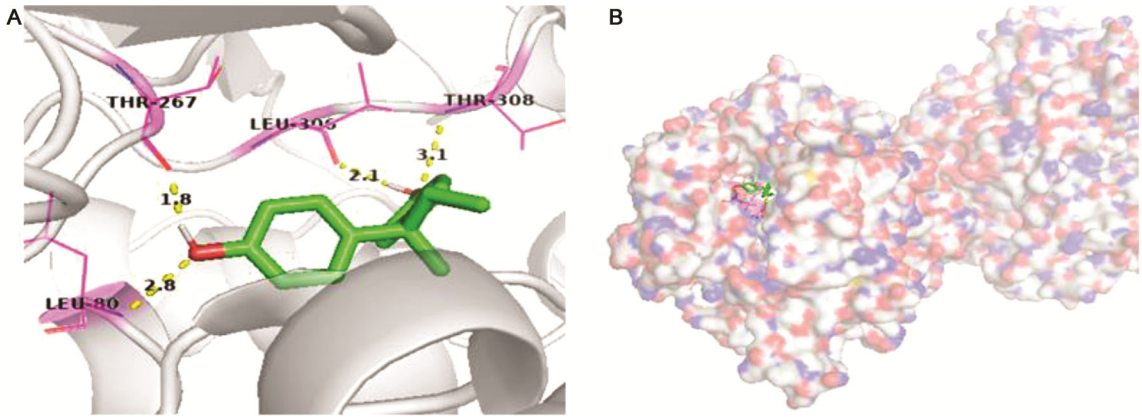

Fig. S10 — Shows the docked complex of Succinate Dehydrogenase protein (grid centre, His 296), bonded with Bisphenol B (BPB, in stick mode) in the cartoon (A) and surface (B) view. BPB interacts with Leu-80, Thr-267, Leu-306 and Thr-308. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

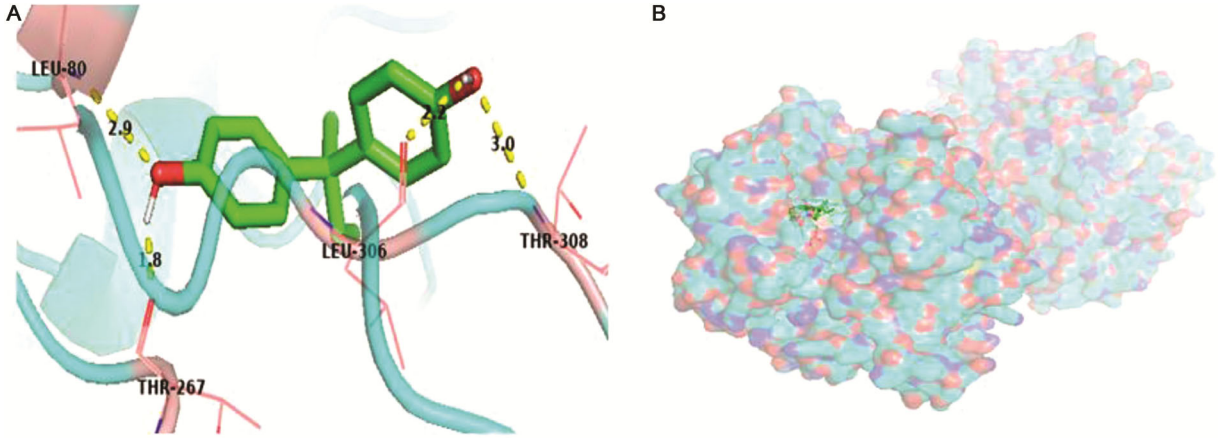

Fig. S11 — Shows the docked complex of Succinate Dehydrogenase protein (grid centre, His 407), bonded with Bisphenol B (BPB, in stick mode) in the cartoon (A) and surface (B) view. BPB interacts with Leu-80, Thr-267, Leu-306 and Thr-308. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labeled along with the residue involved.

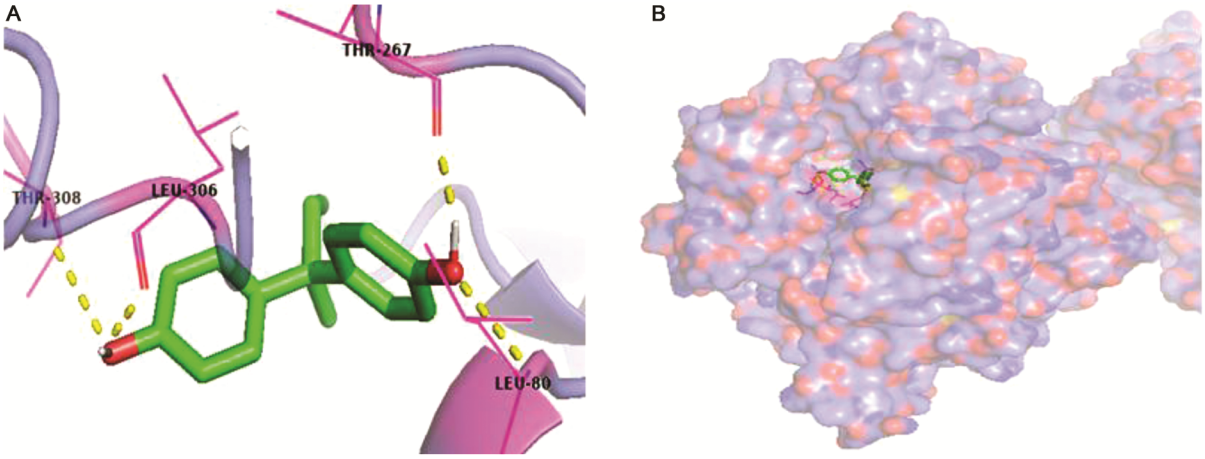

Fig. S12 — Shows the docked complex of Succinate Dehydrogenase protein (grid centre, Thr 308), bonded with Bisphenol B (BPB, in stick mode) in the cartoon (A) and surface (B) view. BPB interacts with Leu-80, Thr-267, Leu-306 and Thr-308. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

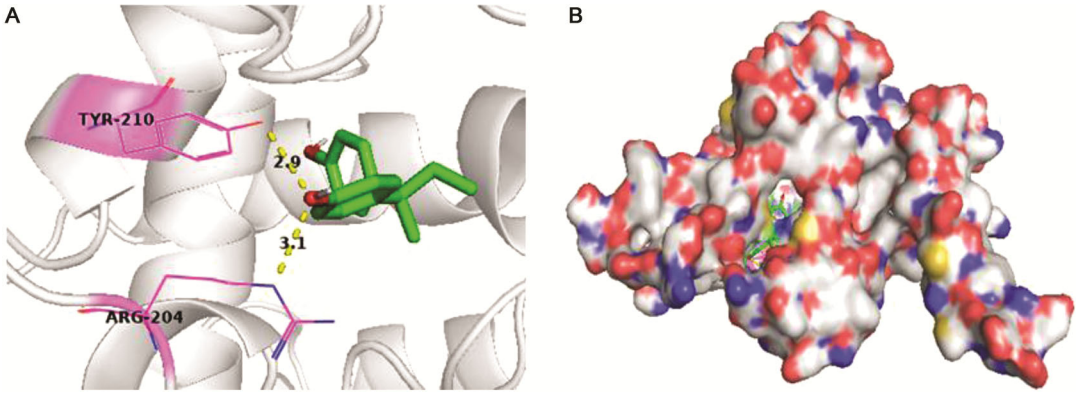

Fig. S13 — Shows the docked complex of Cytochrome B1 Complex protein (grid centre, Cys 121), bonded with Bisphenol B (BPB, in stick mode) in the cartoon (A) and surface (B) view. BPB interacts with Tyr-210 and Arg-204. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

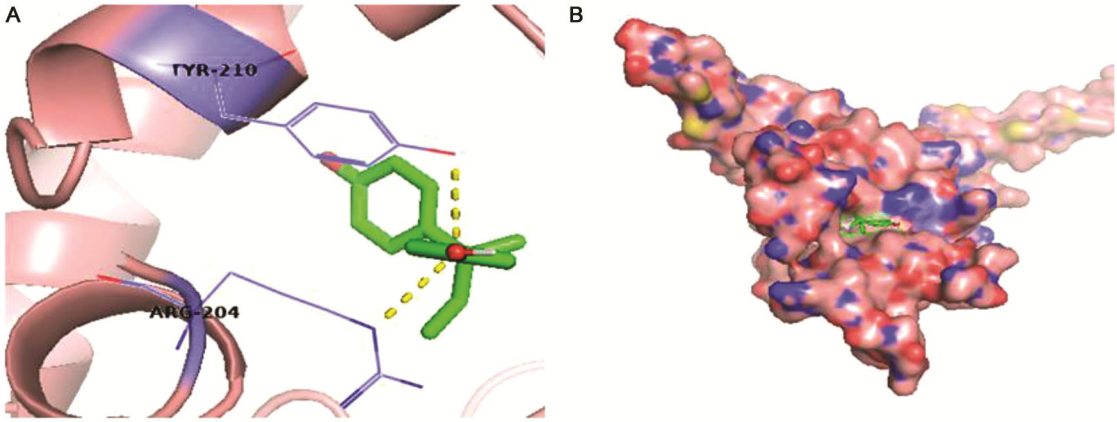

Fig. S14 — Shows the docked complex of Cytochrome B1 Complex protein (grid centre, His 125), bonded with Bisphenol B (BPB, in stick mode) in the cartoon (A) and surface (B) view. BPB interacts with Tyr-210 and Arg-204. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

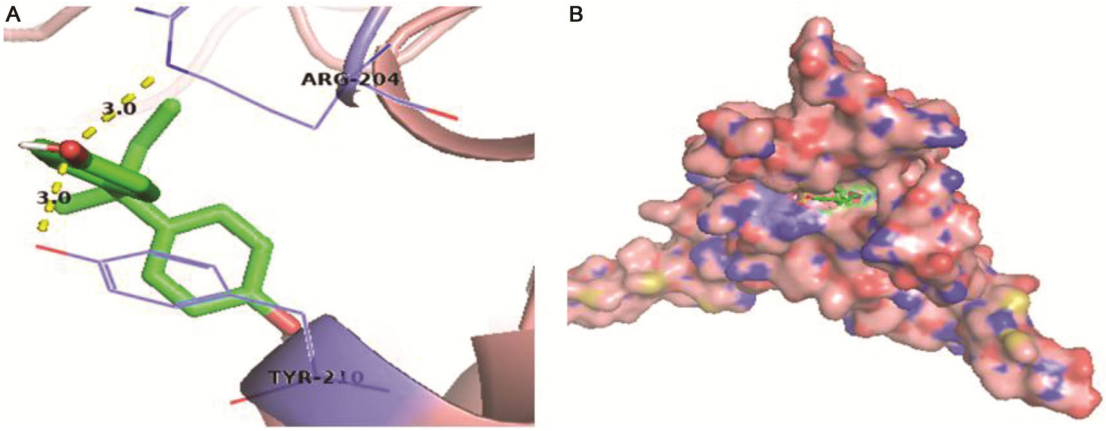

Fig. S15 — Shows the docked complex of Cytochrome B1 Complex protein (grid centre, Met 244), bonded with Bisphenol B (BPB, in stick mode) in the cartoon (A) and surface (B) view. BPB interacts with Arg-204 and Try-210. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

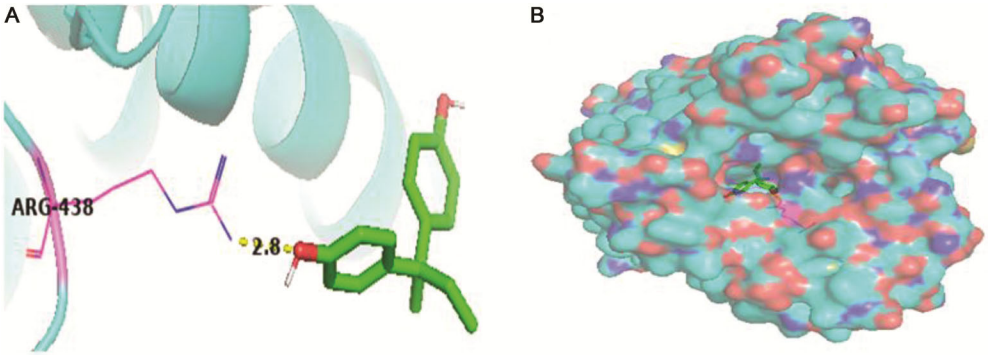

Fig. S16 — Shows the docked complex of Cytochrome C Oxidase protein (grid centre, His 378), bonded with Bisphenol B (BPB, in stick mode) in the cartoon (A) and surface (B) view. BPB interacts with Arg-438. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

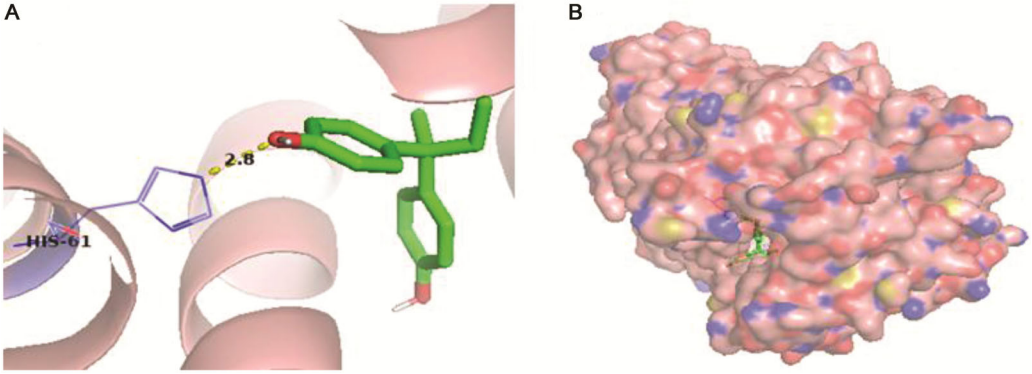

Fig. S17 — Shows the docked complex of Cytochrome C Oxidase protein (grid centre, Ser 382), bonded with Bisphenol B (BPB, in stick mode) in the cartoon (A) and surface (B) view. BPB interacts with His-61. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

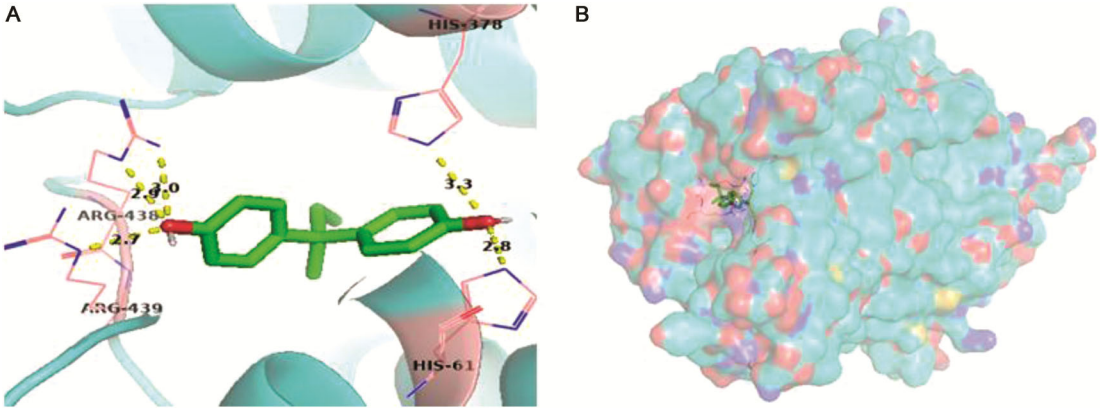

Fig. S18 — Shows the docked complex of Cytochrome C Oxidase protein (grid centre, Tyr 371), bonded with Bisphenol B (BPB, in stick mode) in the cartoon (A) and surface (B) view. BPB interacts with His-61, His-378, Arg-438 and Arg-439. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

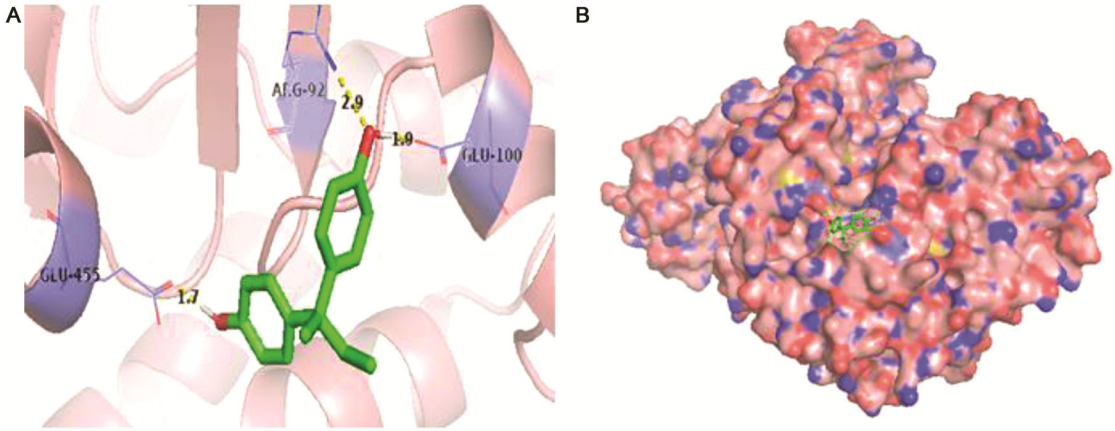

Fig. S19 — Shows the docked complex of Citrate Synthase protein (grid centre, Arg 356), bonded with Bisphenol B (BPB, in stick mode) in the cartoon (A) and surface (B) view. BPB interacts with Arg-92, Glu-100 and Glu-455. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

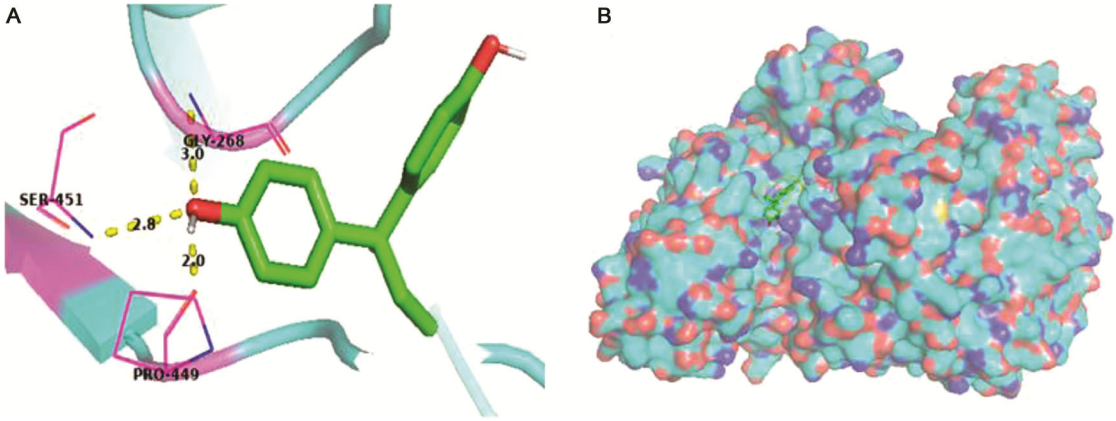

Fig. S20 — Shows the docked complex of Citrate Synthase protein (grid centre, Arg 428), bonded with Bisphenol B (BPB, in stick mode) in the cartoon (A) and surface (B) view. BPB interacts with Gly-268, Pro-440 and Ser-451. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

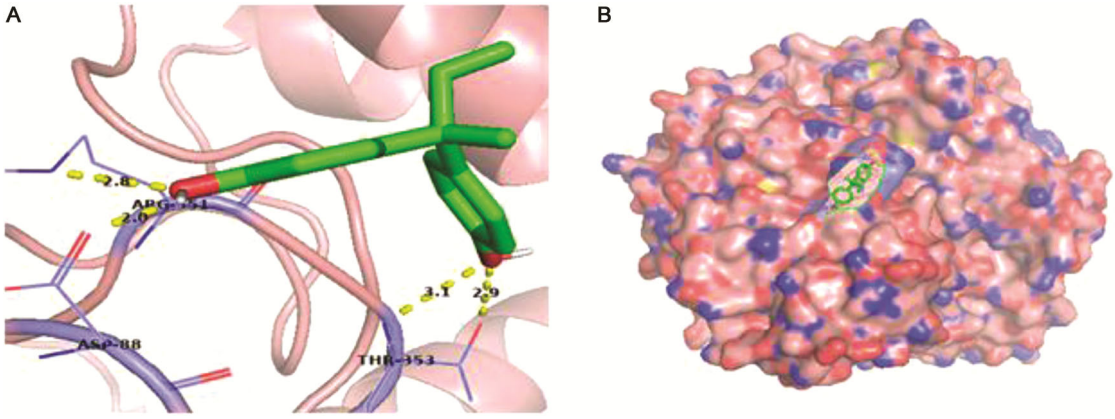

Fig. S21 — Shows the docked complex of Citrate Synthase protein (grid centre, Arg 448), bonded with Bisphenol B (BPB, in stick mode) in the cartoon (A) and surface (B) view. BPB interacts with Asp-88, Arg-351 and Thr-353. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

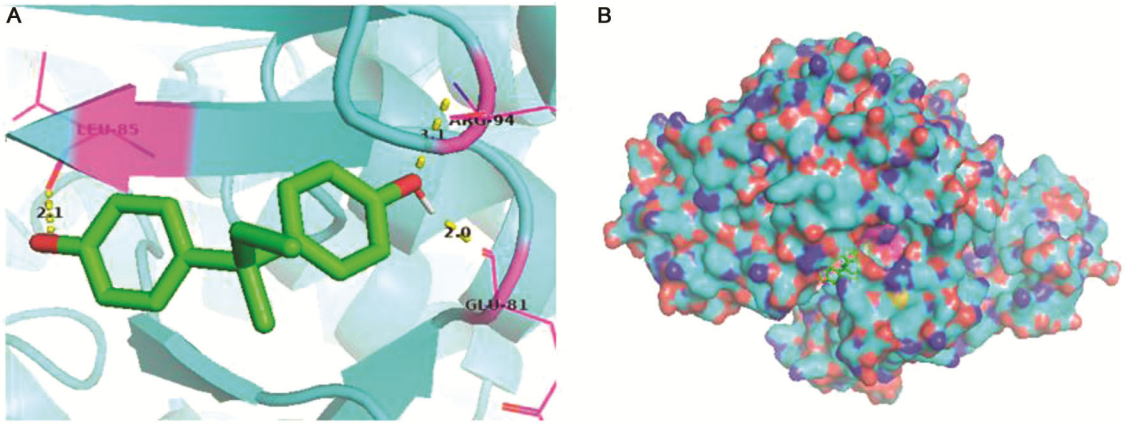

Fig. S22: Shows the docked complex of Citrate Synthase protein (grid centre, His 265), bonded with Bisphenol B (BPB, in stick mode) in the cartoon (A) and surface (B) view. BPB interacts with Glu-81, Leu-85 and Arg-94. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

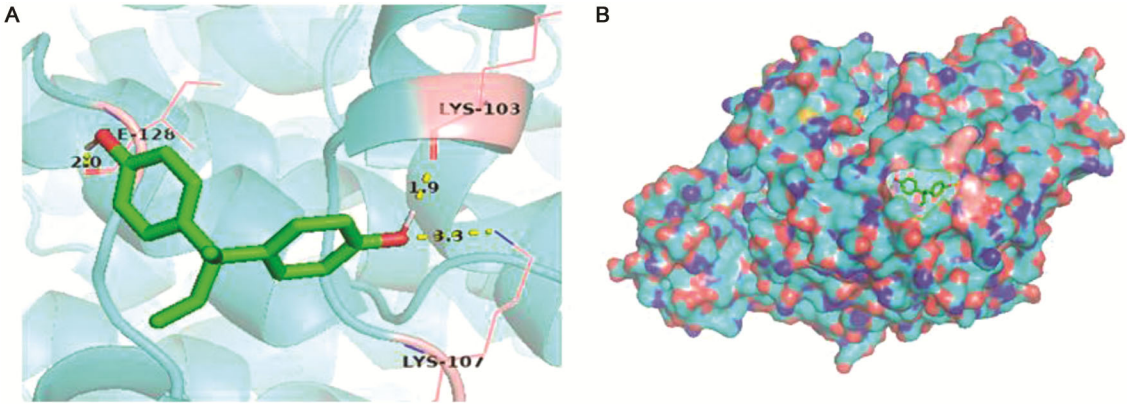

Fig. S23 — Shows the docked complex of Citrate Synthase protein (grid centre, His 347), bonded with Bisphenol B (BPB, in stick mode) in the cartoon (A) and surface (B) view. BPB interacts with Lys-103, Lys-107 and Ileu-128. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

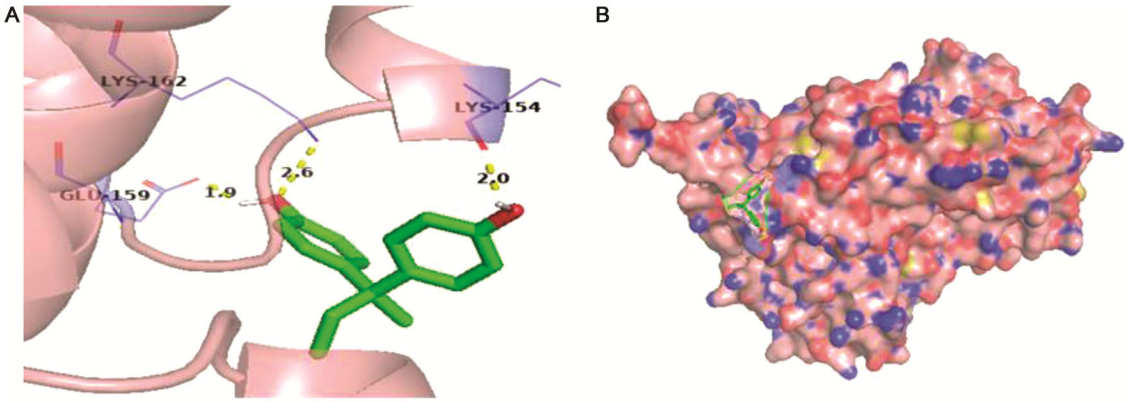

Fig. S24 — Shows the docked complex of Monoamine Oxidase protein (grid centre, Cys 156), bonded with Bisphenol B (BPB, in stick mode) in the cartoon (A) and surface (B) view. BPB interacts with Lys-154, Lys-162 and Glu-159. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

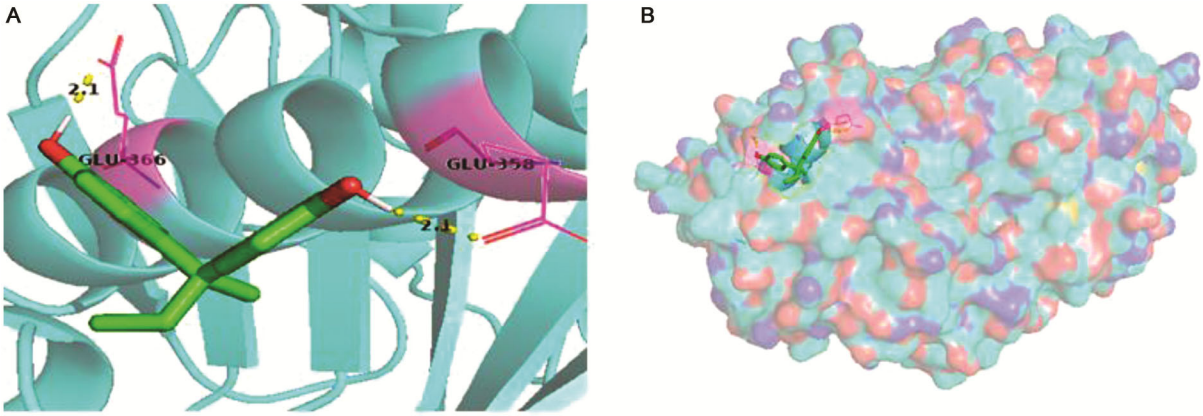

Fig. S25 — Shows the docked complex of Monoamine Oxidase protein (grid centre, Cys 365), bonded with Bisphenol B (BPB, in stick mode) in the cartoon (A) and surface (B) view. BPB interacts with Glu-358 and Glu-366. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

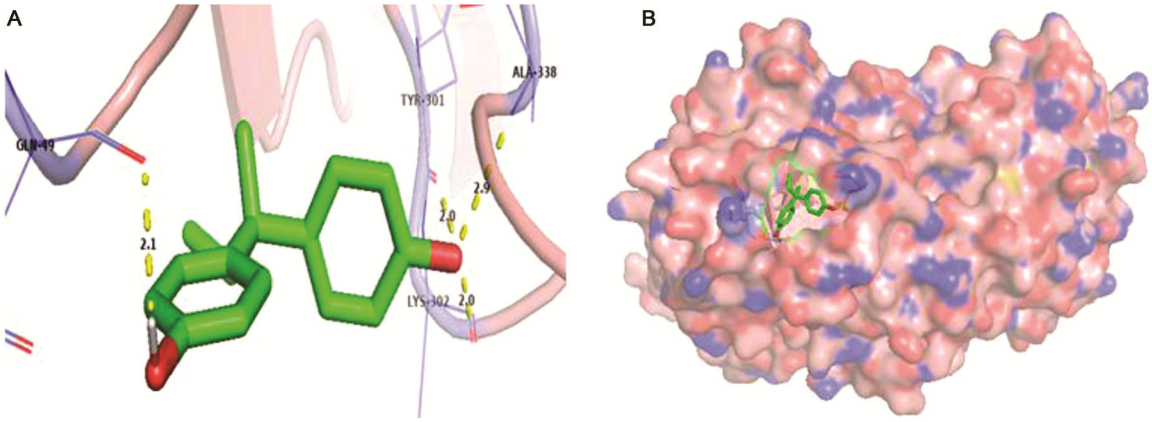

Fig. S26 — Shows the docked complex of Monoamine Oxidase protein (grid centre, His 382), bonded with Bisphenol B (BPB, in stick mode) in the cartoon (A) and surface (B) view. BPB interacts with Gln-49, Tyr-301, Lys-302 and Ala-338. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

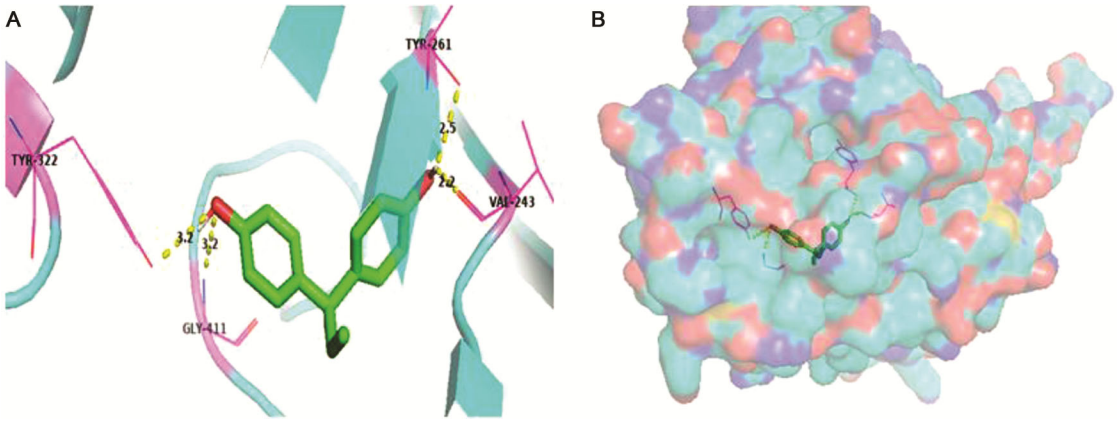

Fig. S27 — Shows the docked complex of Coproporphyrinogen Oxidase protein (grid centre, His 258), bonded with Bisphenol B (BPB, in stick mode) in the cartoon (A) and surface (B) view. BPB interacts with Val-243, Tyr-261, Tyr 322 and Gly-411. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

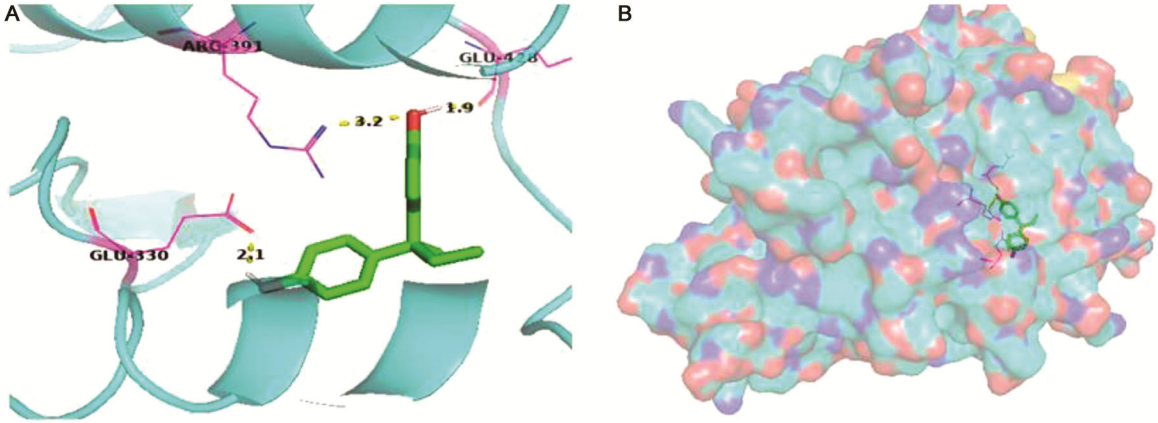

Fig. S28 — Shows the docked complex of Coproporphyrinogen Oxidase protein (grid centre, His 327), bonded with Bisphenol B (BPB, in stick mode) in the cartoon (A) and surface (B) view. BPB interacts with Glu-330, Arg-391 and Glu-428. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved.

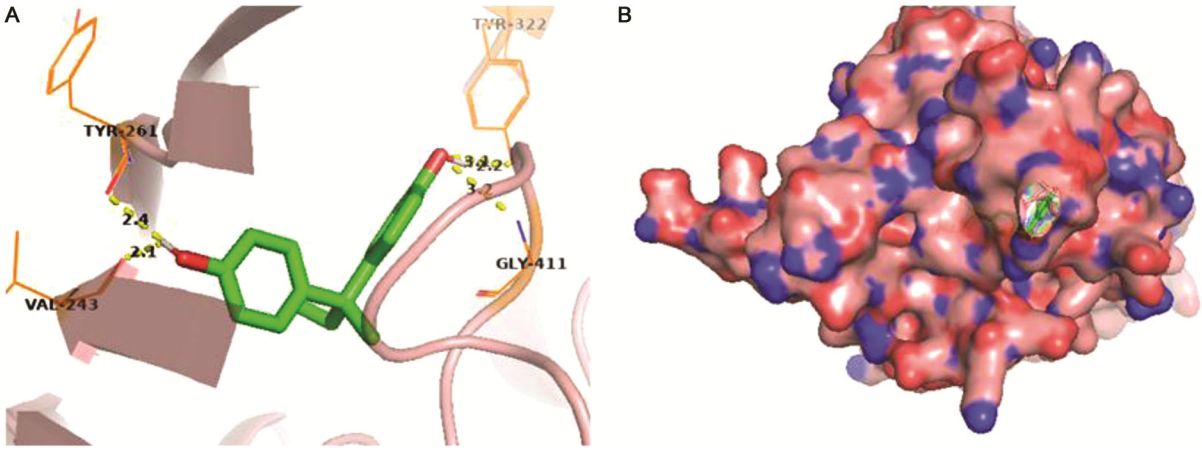

Fig. S29 — Shows the docked complex of Coproporphyrinogen Oxidase protein (grid centre, Ser 244), bonded with Bisphenol B (BPB, in stick mode) in the cartoon (A) and surface (B) view. BPB interacts with Val-243, Tyr-261, Tyr-322 and Gly-411. These dashed lines represent the hydrogen bonds. The bond distances (in Å) are labelled along with the residue involved