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Structure Based Drug Design for Non-Hormonal Male Contraceptives

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Unplanned pregnancies and births can have a devastating socio-economic impact on individuals, families, communities and/or states. The resulting burden of family planning has been placed on women and continues to be so to this day. There is the potential for this burden to be shared by women and men with the advent of additional male contraceptive methods. However, to this date, no pharmaceutical drug, hormonal or non-hormonal, has been approved for use as a male contraceptive world-wide. There are number of ongoing and planned clinical trials for hormonal male contraceptives. In general, the non-hormonal male contraceptives are well behind the hormonal effort. Within the past 5-10 years, more efforts have gone into structure-based drug design (SBDD) of inhibitors for non-hormonal male contraceptive protein targets. Iterative process guided by x-ray co-crystal structure, computational modeling and biochemical and cell-based assays have greatly enhanced the optimization in the development of inhibitors to non-hormonal male contraceptive protein targets. A brief strategy and description of SBDD followed by examples of current research targeting non-hormonal male contraceptive proteins will be presented.