

Fig. S1. Validation of *LY6G6D's* **expression with oncogenes. (A-H)** Validation of the differential expression analysis of *LY6G6D* with established oncogenes in COAD (Normal n=349, Tumor n=275) and READ (Normal n=318, Tumor n=92) tissues via UALCAN, hi-ghlights their potentially dominant role in CRC progression



Fig. S2. Relationship between *LY6G6D* **expression and immune infiltration.** *LY6G6D* expression correlation with immune cells infiltration of (B cells, CD 8+ T cells, CD4 + T cells, Macrophages, Neutrophil and Dendritic cells) are shown in COAD and READ tissues. In COAD, *LY6G6D* exhibits a negative correlation with B cells, CD8+ T cells, macrophages, neutrophils, and dendritic cells, indicating an inverse relationship. Similarly, in READ tissues, B cells, CD8+ T cells, neutrophils, and dendritic cells displays a negative correlation, suggesting immune down-regulation.



Fig. S3. The relative expression of *LY6G6D* in CRC associated with clinicopathological features. UALCAN database was used to assess the expression of *LY6G6D* in comparison with normal to COAD and READ tissues. $P = \le 0.05^*$ (A, B) based on patient's age (C, D) according to three distinct subtypes (E, F) on basis of different stages of CRC



Fig. S4. Kaplan-Meier survival analysis of *LY6G6D.* **(A)** OS did not showed significant difference between high and low expression groups. Log rank p <0.05 was considered statistically significant. **(B)** DFS did not showed significant difference between the expression groups, however the HR = 1.1 suggested a 10% increase in the risk of an event. Log rank p <0.05 was considered statistically significant.

Fig. S5. Evaluation of the robetta generated model 01. **(A)** Z-score shows overall quality of the robetta generated model-01 (-3.72) **(B)** Ramachandran plot of model-01 shows amino acid placement in allowed and disallowed regions with 81.3% in the core region. **(C)** ER-RAT graph showing the correctly and incorrectly determined regions of predicted model-01 with score of 93.04. Two lines (error bars) on the y- axis shows the confidence with which the incorrectly determined regions can be pointed.



Fig. S6. Evaluation of the final refined model (A) A refined 3D structure achieved through the Galaxy Refine server **(B)** Z-score showing overall quality of the final refined 3D model (-3.4) **(C)** Ramachandran plot of final refined 3D model showing amino acid placements in allowed and disallowed regions with 90.7% in the core region. **(D)** ERRAT graph showing the correctly and incorrectly determined regions of the final 3D model with a score of 93.20. Two lines (error bars) on the y- axis shows the confidence with which the incorrectly determined regions can be pointed.



Fig. S7. Evolutionary conservation and binding pocket analysis of LY6G6D (A) Evolutionary conservation analysis of LY6G6D final predicted model is presented in a color coding scheme, which ranges from variable (cyan color) to conserved (maroon color) regions (B) Binding pocket identification of LY6G6D final predicted model by CASTp server. The red highlighted region represents the pocket of interest.

Source articles used to retrive Set B

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