

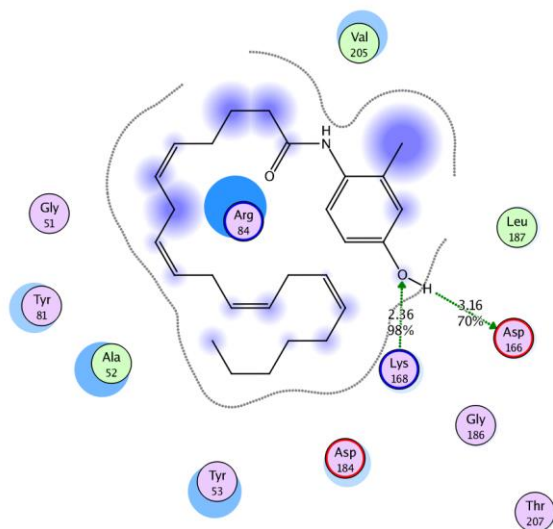
## SUPPLEMENTARY DATA

**Table S1: Name of overlapping genes with their possible functions**

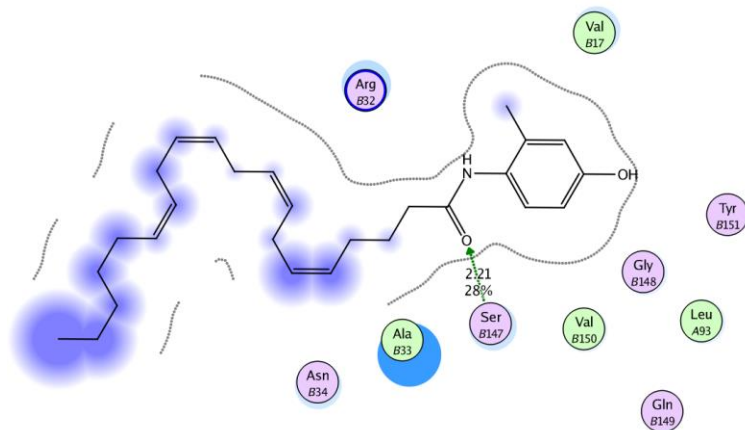
| Gene    | Gene Name  | Possible Function  |
|---------|--|--|
| CPHR1   | Corticotropin Releasing Hormone Receptor 1                             | Regulates diverse physiological processes including obesity, stress, immune response and reproduction  |
| NR3C1   | Nuclear Receptor Subfamily 3 Group C Member 1                          | Regulates cellular proliferation, inflammatory responses and differentiation in target issues  |
| HTR2A   | 5-Hydroxytryptamine Receptor 2A  | Regulates disorder including Major Depressive Disorder and Obsessive-Compulsive Disorder.  |
| L1B     | Interleukin-1 Beta   | involved in a variety of cellular activities, including cell proliferation, differentiation, and apoptosis   |
| CNR1    | Cannabinoid Receptor 1   | Mediates CNS effects including alterations in mood and cognition   |
| MAOA    | Monoamine Oxidase A  | associated with a variety of psychiatric disorders, including antisocial behavior  |
| NR3C2   | Nuclear Receptor Subfamily 3 Group C Member 2                          | mediates aldosterone actions on salt and water balance within restricted target cells  |
| TNF     | Tumor Necrosis Factor  | Involved in the regulation of a wide spectrum of biological processes including cell proliferation, differentiation, apoptosis, lipid metabolism, and coagulation.   |
| GFAP    | Glial Fibrillary Acidic Protein  | Plays role in pathophysiology of Alexander Disease and Central Neurocytoma.  |
| CNR2    | Cannabinoid Receptor 2   | Mediates CNS effects including alterations in mood and cognition   |
| MAPK3   | Mitogen-Activated Protein Kinase 3                                     | regulates various cellular processes such as proliferation, differentiation, and cell cycle progression in response to a variety of extracellular signals  |
| HTR4    | 5-Hydroxytryptamine Receptor 4   | This gene functions in both peripheral and central nervous system to modulate the release of various neurotransmitters   |
| PFKFB3  | 6-Phosphofructo-2-Kinase/Fructose-2,6-Biphosphatase 3                  | Involved in cell cycle progression and prevention of apoptosis.  |
| ALK     | ALK Receptor Tyrosine Kinase   | Regulates brain development, tumourigenesis  |
| GRPR    | Gastrin Releasing Peptide Receptor                                     | Regulates release of gastrointestinal hormones, smooth muscle cell contraction, and epithelial cell proliferation and is a potent mitogen for neoplastic tissues   |
| ESR2    | Estrogen Receptor 2  | Controls growth, differentiation and function of the reproductive system, growth and maintenance of the skeleton and the normal function of the cardiovascular and nervous systems.  |
| NPY1R   | Neuropeptide Y Receptor Y1   | mediate a diverse range of biological actions including stimulation of food intake and modulation of circadian rhythm  |
| ACE     | Angiotensin converting enzyme  | catalyzes the conversion of angiotensin I into a physiologically active peptide angiotensin II and have evident role in pathophysiology of various disorders including cardiovascular pathophysiology's, psoriasis, renal disease, stroke, and Alzheimer's disease |
| PIK3CG  | Phosphatidylinositol-4,5-Bisphosphate 3-Kinase Catalytic Subunit Gamma | Involved in the immune response  |
| MAPK1   | Mitogen-Activated Protein Kinase 1                                     | Involved in a wide variety of cellular processes such as proliferation, differentiation, transcription regulation and development.   |
| AGTR1   | Angiotensin II Receptor Type 1   | mediates major cardiovascular effects of angiotensin II  |
| PPARG   | Peroxisome Proliferator Activated Receptor Gamma                       | a regulator of adipocyte differentiation and has been implicated in the pathology of numerous diseases including obesity, diabetes, atherosclerosis and cancer   |
| ADORA2A | Adenosine A2a Receptor   | plays an important role in many biological functions, such as cardiac rhythm and circulation, cerebral and renal blood flow, immune function, pain regulation, and sleep   |
| MTOR    | Mechanistic Target Of Rapamycin Kinase                                 | Mediate cellular responses to stresses such as DNA damage and nutrient deprivation.  |
| BCL2    | BCL2 Apoptosis Regulator   | blocks the apoptotic death of some cells such as lymphocytes   |
| BMP1    |  |  |
| GRIN1   | Glutamate Ionotropic Receptor NMDA Type Subunit 1                      | play a key role in the plasticity of synapses, which is believed to underlie memory and learning   |

|         |  |  |
|---------|--|--|
| IGF1R   | Insulin Like Growth Factor 1 Receptor              | plays a critical role in transformation events   |
| CDK7    | Cyclin Dependent Kinase 7                          | important regulators of cell cycle progression   |
| CPT1A   | Carnitine Palmitoyltransferase 1A                  | Regulation of fatty acid beta-oxidation  |
| ALDH2   | Aldehyde Dehydrogenase 2 Family Member             | Required for clearance of cellular formaldehyde, a cytotoxic and carcinogenic metabolite that induces DNA damage   |
| ALOX5   | Arachidonate 5-Lipoxygenase                        | plays a dual role in the synthesis of leukotrienes from arachidonic acid   |
| ALOX5   | Arachidonate 5-Lipoxygenase                        | required for leukotriene synthesis   |
| AP      | Activating Protein                                 |  |
| HPGDS   | Hematopoietic Prostaglandin Synthase               | plays a role in the production of prostanoids in the immune system and mast cells  |
| FFAR1   | Free Fatty Acid Receptor 1                         | involved in the metabolic regulation of insulin secretion  |
| INSR    | Insulin Receptor                                   | Binding of insulin or other ligands to this receptor activates the insulin signaling pathway, which regulates glucose uptake and release, as well as the synthesis and storage of carbohydrates, lipids and protein        |
| IL2     | IL2 Inducible T Cell Kinase                        | play a role in T-cell proliferation and differentiation  |
| ME1     | Malic Enzyme 1                                     | links the glycolytic and citric acid cycles  |
| MIF     | Macrophage Migration Inhibitory Factor             | involved in cell-mediated immunity, immunoregulation, and inflammation   |
| MMP12   | Matrix Metalloproteinase 12                        | involved in the breakdown of extracellular matrix in normal physiological processes, such as embryonic development, reproduction, and tissue remodeling, as well as in disease processes, such as arthritis and metastasis |
| PLA2G2A | Phospholipase A2 Group IIA                         | targets extracellular phospholipids with implications in host antimicrobial defense, inflammatory response and tissue regeneration   |
| PRCP    | Prolylcarboxypeptidase                             | Mature lysosomal prolylcarboxypeptidase, linked to proline in peptides such as angiotension II, III and des-Arg9-bradykinin.   |
| SOAT1   | Sterol O-Acyltransferase 1                         | implicated in the formation of beta-amyloid and atherosclerotic plaques by controlling the equilibrium between free cholesterol and cytoplasmic cholesteryl esters   |
| STAT6   | Signal Transducer And Activator Of Transcription 6 | Involved in IL4/interleukin-4- and IL3/interleukin-3-mediated signaling  |
| TACR3   | Tachykinin Receptor 3                              | associated with G proteins that activate a phosphatidylinositol-calcium second messenger system  |
| CAPN2   | Calpain 2  | involved in cytoskeletal remodeling and signal transduction  |

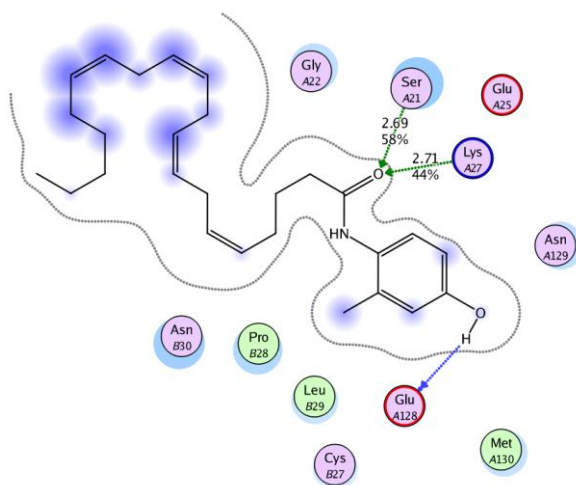
Figure S1a: Molecular docking of VDM11 with selected targets



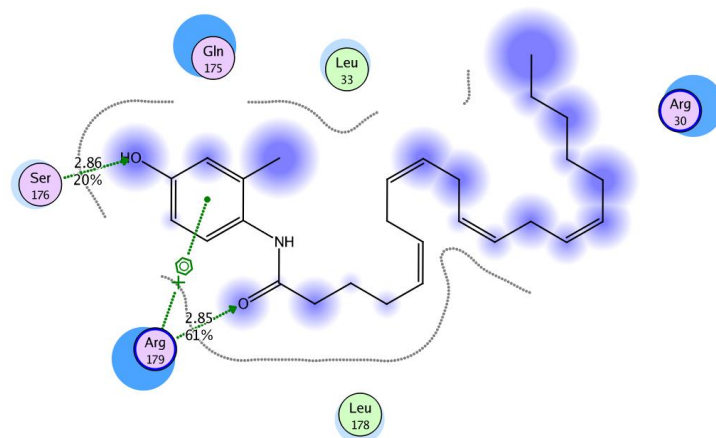
#### VDM11-MAPK3 INTERACTION



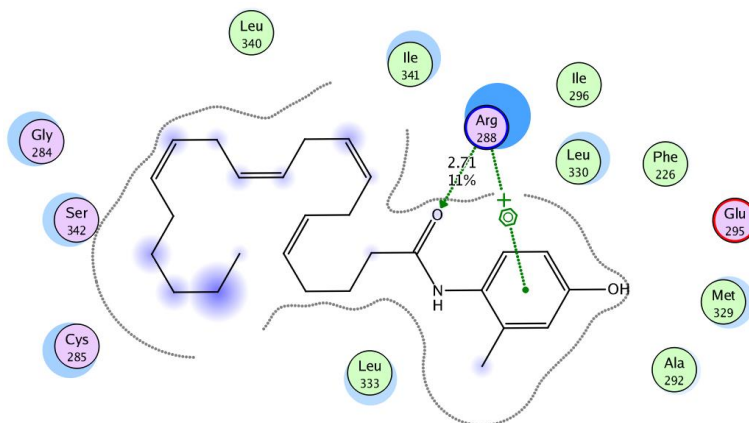
#### VDM11-TNF-α INTERACTION



#### VDM11-IL1B INTERACTION

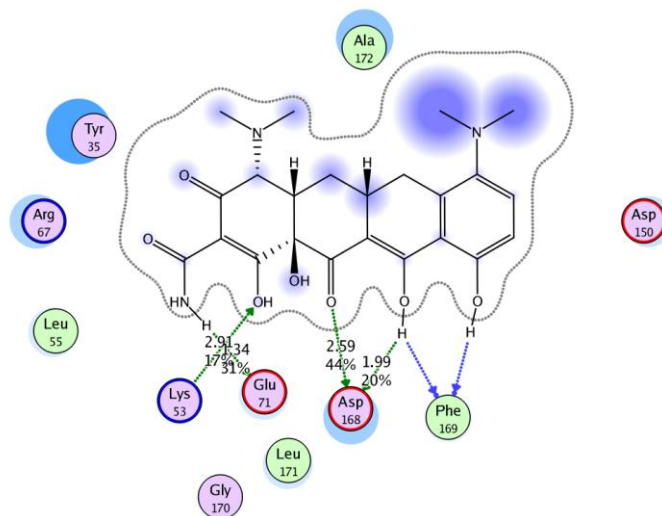


### VDM11-IL6 INTERACTION

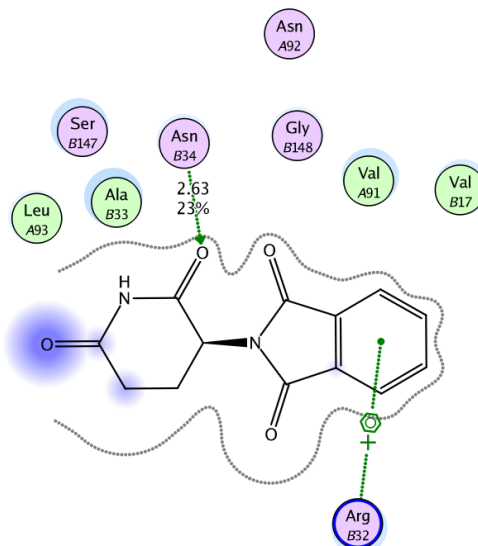


### VDM11-IL6 INTERACTION

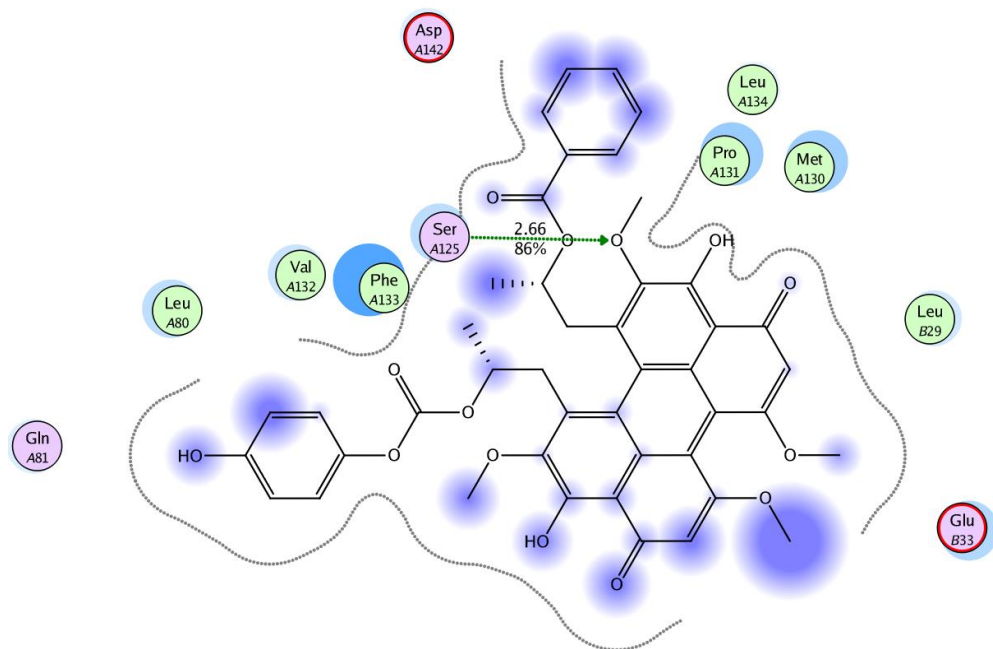
Figure S1b: Binding mode representation of positive controls with selected targets



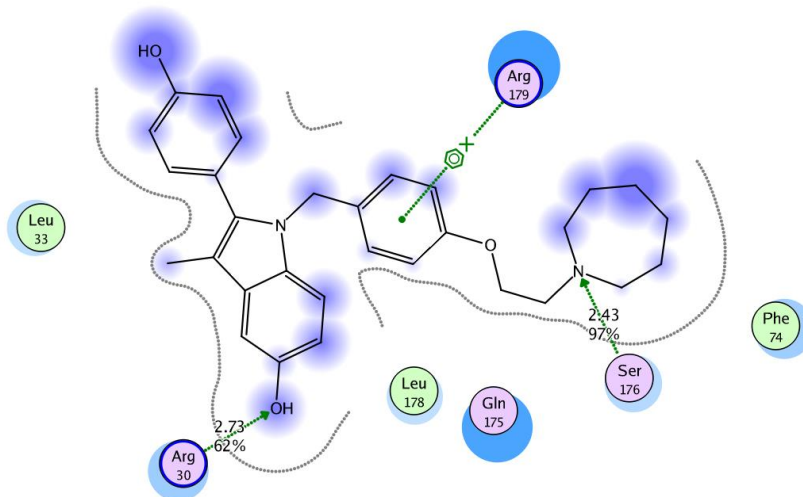
Minocycline-MAPK3 Interaction



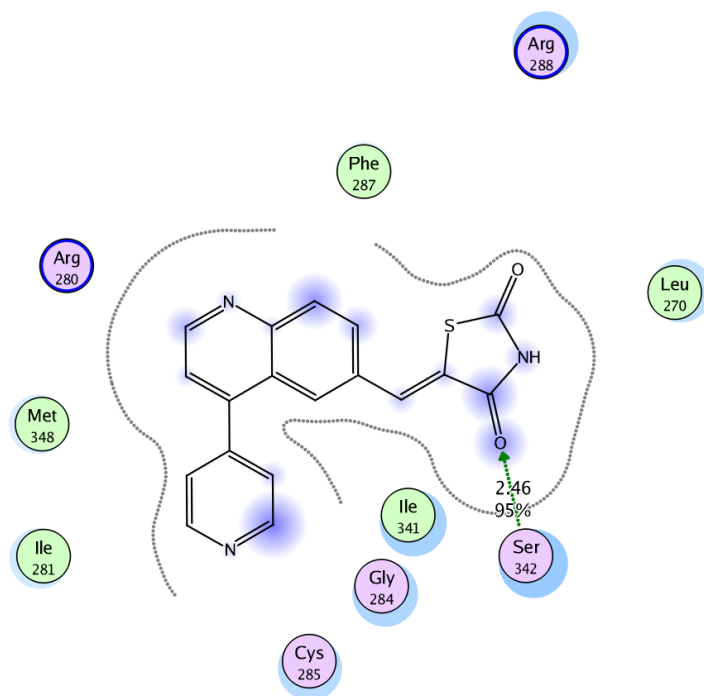
Thalidomide-TNF Interaction



**PKF115-584-IL1B Interaction**



**Bazedoxifene-IL6 Interaction**



**Thiazolidenedione-PPARG Interaction**