Inhibiton of NFκB activation and aromatase activity by vanilloids: An *in vitro* and *in silico* study

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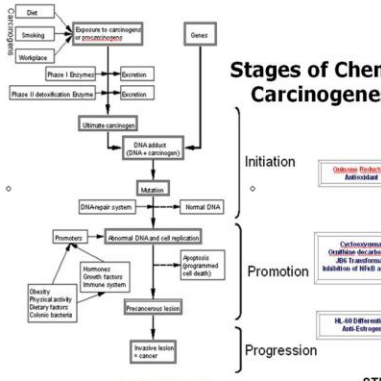
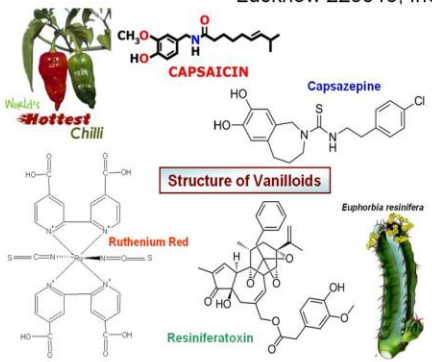
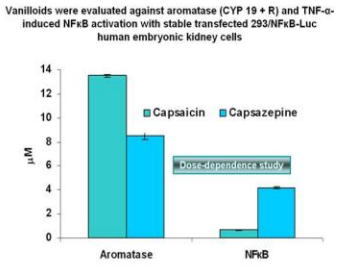
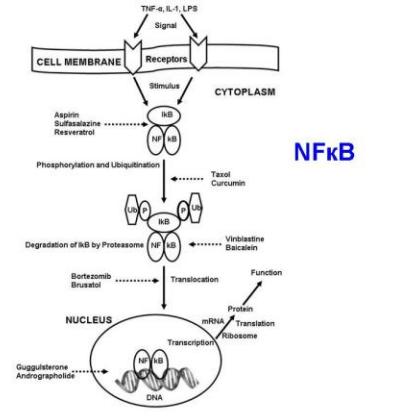
Nature Precedings : doi:10.1038/npre.2012.6913.1 : Posted 22 Feb 2012



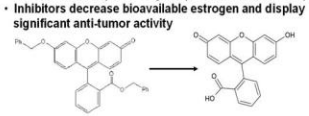




Aromatase assay: Maiti *et al.*, (2007)
NFκB Luciferase Reporter Assay: Homhual *et al.*, (2006)
Cytotoxicity by SRB Assay: Skehan P *et al.*, (1990)



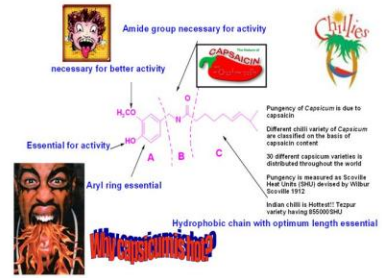
- Cytochrome P450 (CYP19)
- Aromatizes androgens (testosterone and androstenedione) to estrogens (estradiol and estrone)
- Inhibitors decrease bioavailable estrogen and display significant anti-tumor activity

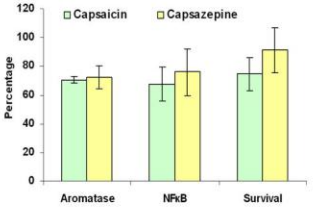


Aromatase converts dibenzylfluorescein to fluorescein

Inhibition can be determined by measuring fluorescence

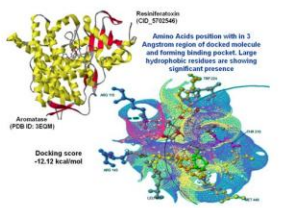
STRUCTURE AND ACTIVITY RELATIONSHIP OF CAPSAICIN

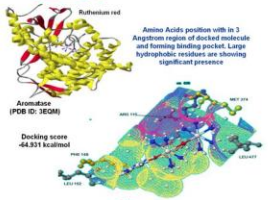


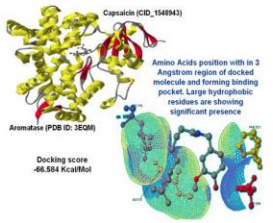


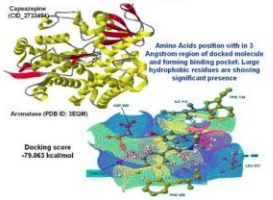
Receptor: Ligand	AROMATASE (PDB ID 3EQM)		NFκ B2 (PDB ID 2D96)		NF κB1 (PDB ID 1BFS)		ORNITHINE DECARBOXYLASE (PDB ID 1D7K)		QUINONE REDUCTASE 2 (PDB ID 1QR2)		QUINONE REDUCTASE 1 (PDB ID 1GGS)	
	PMF	AA	PMF	AA	PMF	AA	PMF	AA	PMF	AA	PMF	AA
Capsaicin (CID_1548943)	-64.584	ARG-115, ILE-133, PHE-221, ASP-309	-53.01	VAL-96, ARG-97, ARG-99	-35.71	GLN-279, PHE-295, ASP-297, LYS-334	102.57	ASP-88, ARG-154, PHE-170, HIS-197, SER-200, ARG-277, TYR-221, ASP-332, TYR-389	65.89	LYS-113, ASP-117, LEU-120, PHE-125, PHE-178	-63.57	LYS-113, PHE-116, GLU-117, PHE-120, PRO-170, ILE-171, ILE-175, PHE-178
capsazepine (CID_2733484)	-79.063	ILE-113, PHE-134, ASP-309, THR-310, VAL-371, LEU-372, PHE-430, LEU-477, SER-478	-57.47	GLU-93, VAL-96, ARG-97, ARG-99	-49.08	GLN-279, GLU29 3, PHE-295, ASP-297, ARG-302, LYS-334	-97.22	ASP-88, PHE-170, ARG-154, HIS-197, SER-200, GLU-274, ARG-277, ASP-332, TYR-389	65.87	MET-116, LEU-120, GLY-174, THR-175, PHE-125, PHE-178	-77.60	PHE-120, TYR-126, TRY-102, ILE-175, PHE-178, CYS-179

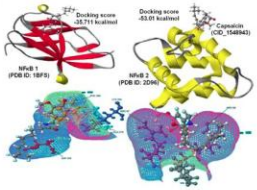
Note:
AA (3A°) Amino Acids position with in 3 Angstrom region of docked molecule and forming binding pocket. Red coloured amino acid indicates conservation & thus found in all pockets.
PMF Potential Mean Force value as docking score in Kcal/mol unit.
Docking score in negative value means good interaction (low energy) between bioactive chemical molecule and targetreceptor. Positive docking score indicates poor interaction energy, thus should be rejected as potential targetreceptor.
Highlight amino acid are the common amino acid showing bind with all lead molecule with respect to each receptor.

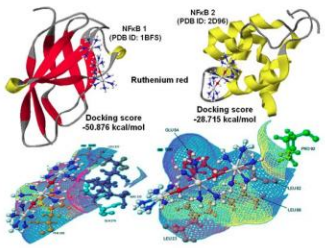


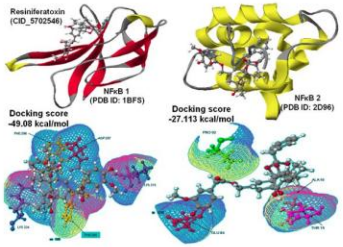


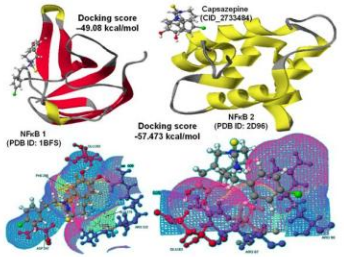












ACKNOWLEDGEMENT SL acknowledge Indo-US Science and Technology Forum (IUSSTF), New Delhi for Research Fellowship. Work supported by program project P01 CA048112 awarded by the National Cancer Institute.

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