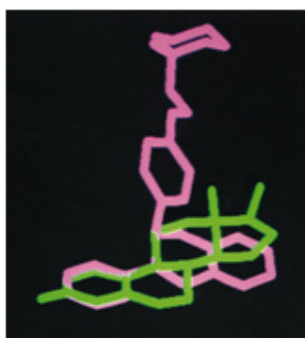


## Design, synthesis of benzopyrans and computer aided insight into their SERM type activities

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Since more than two decades our efforts in the design and development of Selective Estrogen Receptor Modulators (SERMs) have resulted in the access of 2, 3-diaryl-2H-1-benzopyrans (DABPs) as a promising new class of non-steroidal molecules possessing significant anti-estrogenic activities. A series of these compounds with different substituent patterns were synthesized and in particular, most of these showed extremely high post-coital contraceptive activity at very low doses. Extensive biological studies indicated that these molecules also exhibit tissue selective effects acting as agonists on bone and cardiovascular systems while antagonizing the effects of estrogen on uterine and breast tissues and, therefore, have been termed as selective estrogen receptor modulators. *In silico* analysis of 3-D overlay model of one of our lead structures and estradiol for estrogen receptor binding revealed that the active enantiomer would bind to the receptor in a fashion such that the tertiary amino alkoxy phenyl residue would occupy a region corresponding to the 11b-position of the estradiol. This would be possible only if the pendant aryl ring at 3-position overlays on to the aromatic A ring of the benzopyran.



Detailed account of Design, Synthesis of Benzopyrans and Computer Aided Insight into Their SERM Type Activities will be discussed.

### Biography

Jaya Pandey has completed her Ph.D. from Central Drug Research Institute, Lucknow and she is presently working as an Assistant Professor at Amity University. She has experience of being a research fellow at Medicinal Chemistry Division in CDRI and NBRI, Lucknow during her Ph.D. and post-Ph.D. dissertations. She is also conferred with two prestigious 'Young Scientist Awards' by the "Indian council of Chemists" and "Indian Chemical Society", respectively for her excellent scientific contribution to the fields of medicinal/organic chemistry. Her work has mainly been associated with a development of new diarylbenzopyrans (DABPs) as Selective Estrogen Receptor Modulators (SERMs).

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