First chemical feature-based pharmacophore modeling of potent retinoidal retinoic acid metabolism blocking agents (RAMBAs): identification of novel RAMBA scaffolds.
Title: First chemical feature-based pharmacophore modeling of potent retinoidal retinoic acid metabolism blocking agents (RAMBAs): identification of novel RAMBA scaffolds.

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Abstract: The first three-dimensional (3D) pharmacophore model was developed for potent retinoidal retinoic acid metabolism blocking agents (RAMBAs). This model is based on the three-dimensional fingerprint of potent structurally diverse retinoidal retinoic acid metabolism blocking agents. The model is generated with the help of upgrade of a publicly available 3D pharmacophore database. The developed 3D pharmacophore model is suitable for virtual screening of libraries by means of 3D QSAR docking and searches of other robust databases is currently in progress with a view to identifying and optimizing new leads.

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