

FieldStere: Application to the Discovery of 5HT_{1D} Agonists

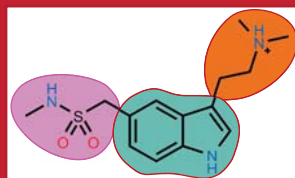
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Application of FieldStere to 5HT_{1D} Agonists



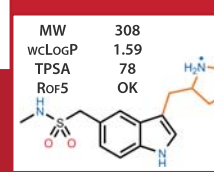
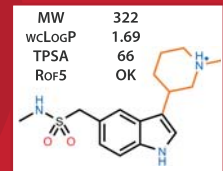
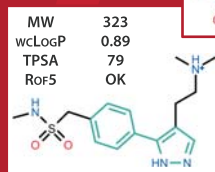
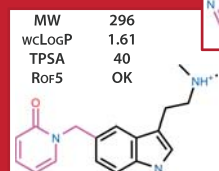
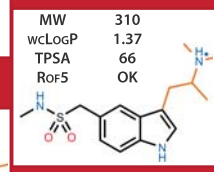
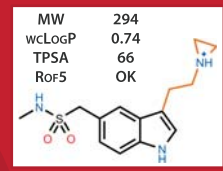
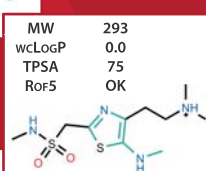
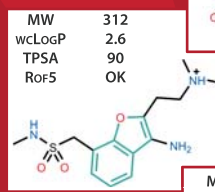
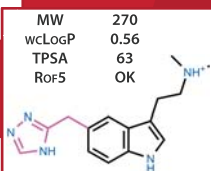
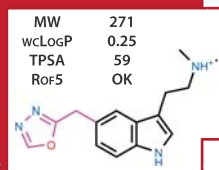
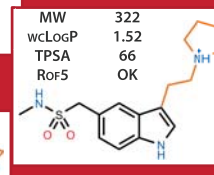
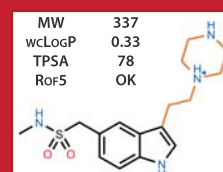
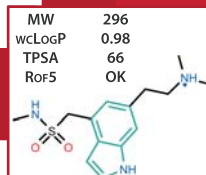
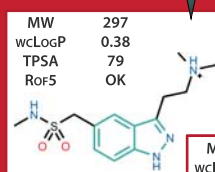
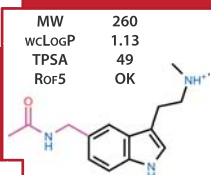
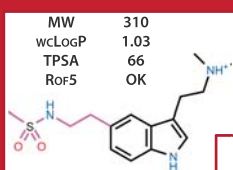
MW 296
wcLogP 0.98
TPSA 66
RoF5 OK

fieldstere™

Obvious

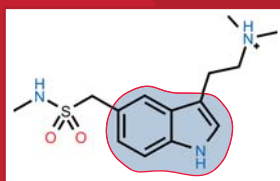
Less Obvious

Non Obvious



FieldStere Operation

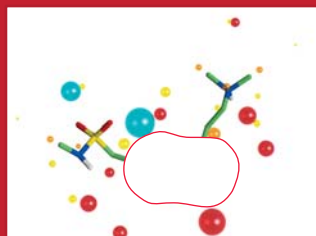
KNOWN ACTIVE LIGAND



BIOISOSTERE SEARCH

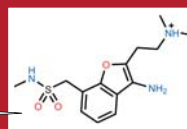
SELECT PORTION OF MOLECULE FOR WHICH BIOISOSTERES ARE REQUIRED

CONVERT TO 3D
ADD FIELDS
REMOVE UNWANTED ATOMS

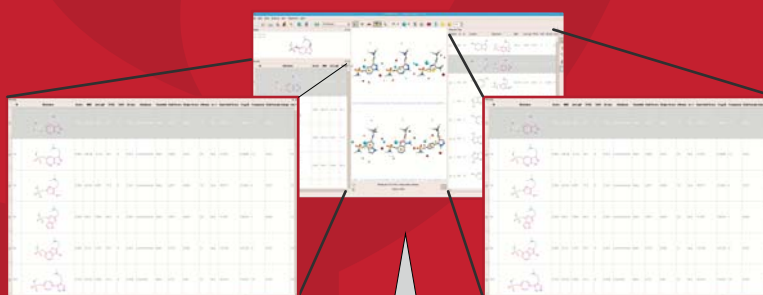


DATABASE OF 200,000 FRAGMENTS FROM COMMERCIAL COMPOUNDS

SEARCH FOR REPLACEMENTS WITH SIMILAR FIELD PATTERN



FORM NEW MOLECULE



ADD RELEVANT PHYSICAL PROPERTIES
CLUSTER RESULTS

POTENTIAL BIOISOSTERES ARE SCORED AS PRODUCT MOLECULES
ADVANTAGES:

CONTEXT SENSITIVE SCORING
MORE DIVERSITY
COOPERATIVITY TAKEN INTO ACCOUNT