

Supporting Information

Insights into Drug Cardiotoxicity from

Biological and Chemical Data: The

First Public Classifiers for FDA

DICTrank

*Srijit Seal^{*1}, Ola Spjuth², Layla Hosseini-Gerami³, Miguel García-Ortegón⁴, Shantanu Singh¹,
Andreas Bender⁴, Anne E. Carpenter¹*

¹Imaging Platform, Broad Institute of MIT and Harvard, Cambridge, MA 02142, US

²Department of Pharmaceutical Biosciences and Science for Life Laboratory, Uppsala University, Box 591, SE-75124, Uppsala, Sweden

³ Ignota Labs, County Hall, Westminster Bridge Rd, SE1 7PB, London, United Kingdom

⁴ Yusuf Hamied Department of Chemistry, University of Cambridge, Lensfield Rd, CB2 1EW, Cambridge, United Kingdom

Documentation: https://broad.io/DICTrank_Predictor

Code: <https://github.com/srijitseal/DICTrank>

Datasets: 10.6084/m9.figshare.24312274

*Correspondence:

seal@broadinstitute.org

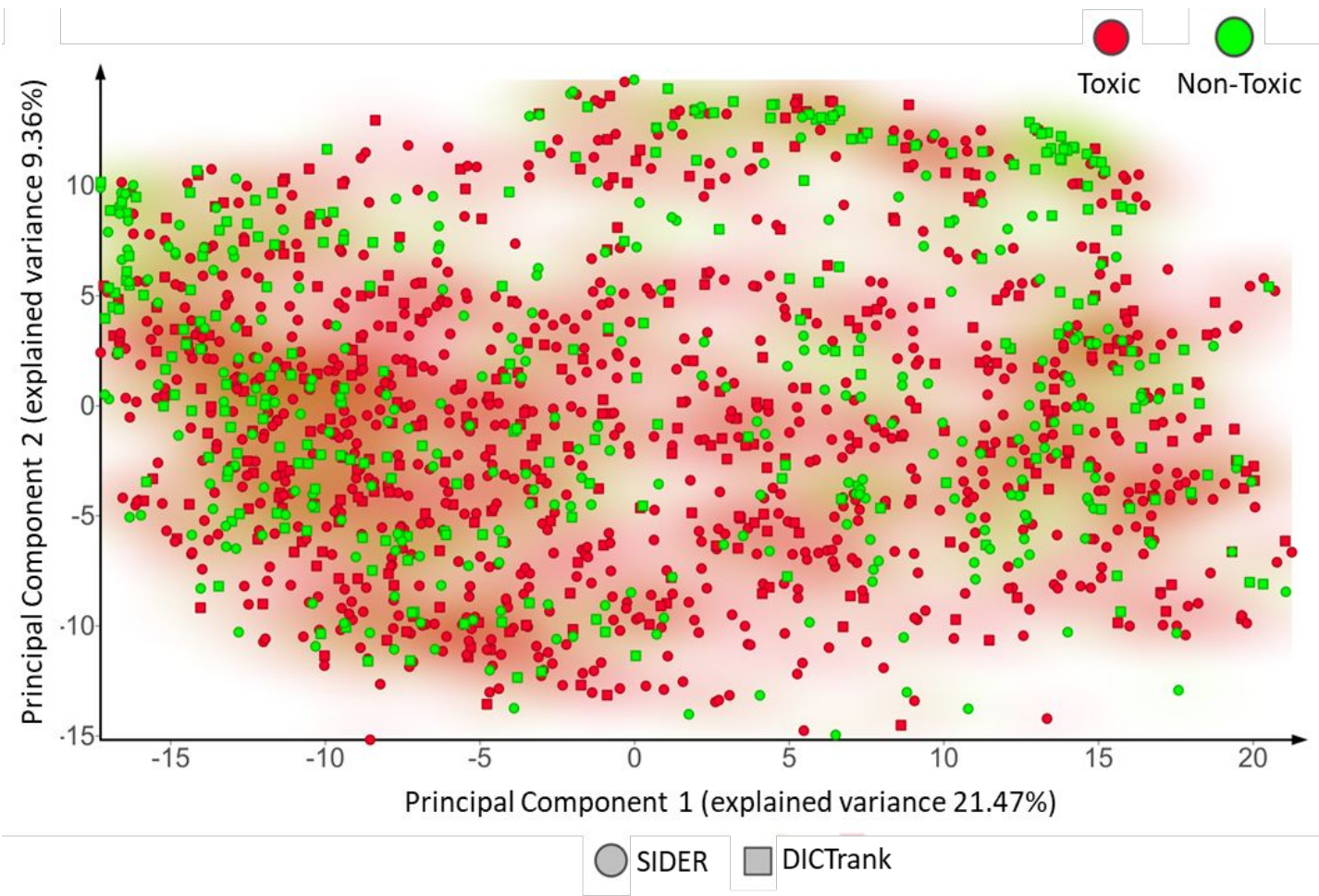
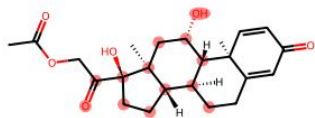


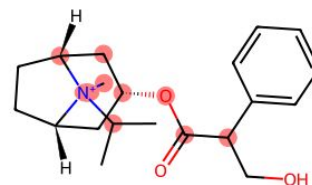
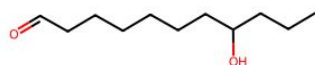
Figure S1: The chemical space of all 1020 DICTrank compounds and the remaining 546 unique compounds in SIDER as defined by FragFP fingerprints (chemical fingerprints) in a principal component analysis. SIDER and DICTrank compounds fairly overlap (with the PCA explained variance of 21.47%).



prednisolone acetate

['Cardiac disorders']

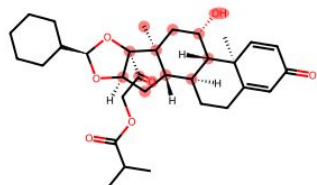
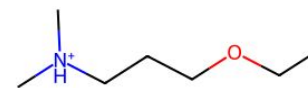
Additional Data: ['approved']



ipratropium

['Cardiac disorders']

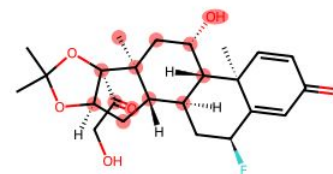
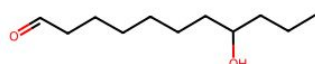
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ciclesonide

['Cardiac disorders']

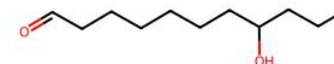
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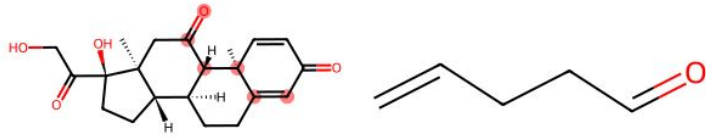


flunisolide

['Cardiac disorders']

Additional Data: ['approved', 'investigational']

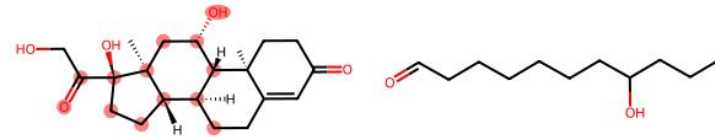




prednisone

['Cardiac disorders']

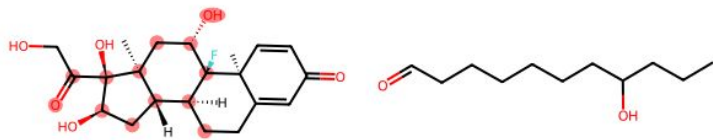
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hydrocortisone

['Cardiac disorders']

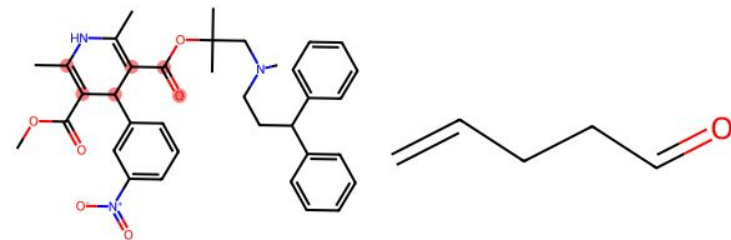
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triamcinolone

['Cardiac disorders']

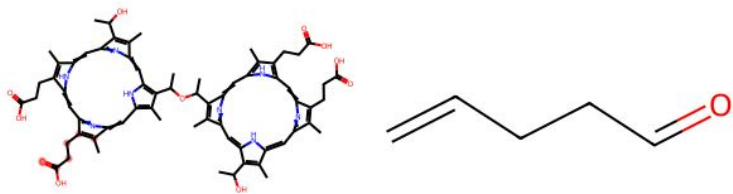
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lercanidipine

['Cardiac disorders']

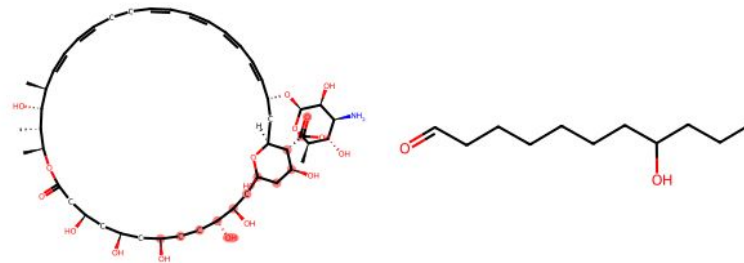
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dihematoporphyrin ether

['Cardiac disorders']

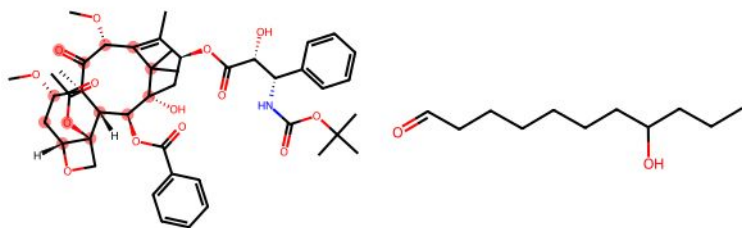
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nystatin

['Cardiac disorders']

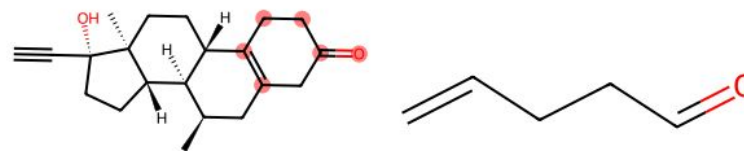
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cabazitaxel

['Cardiac disorders']

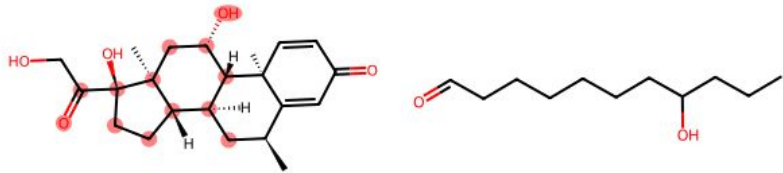
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tibolone

['Cardiac disorders']

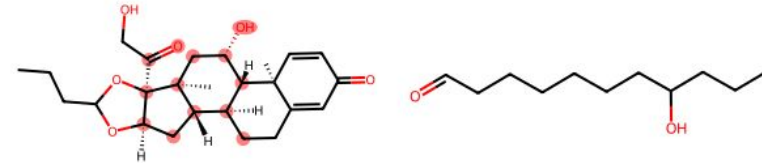
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methylprednisolone

['Cardiac disorders']

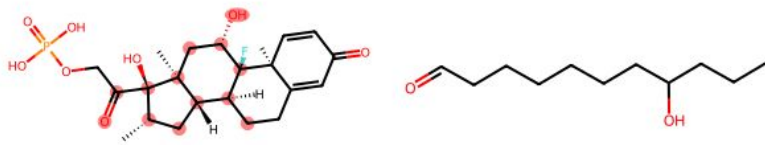
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budesonide

['Cardiac disorders']

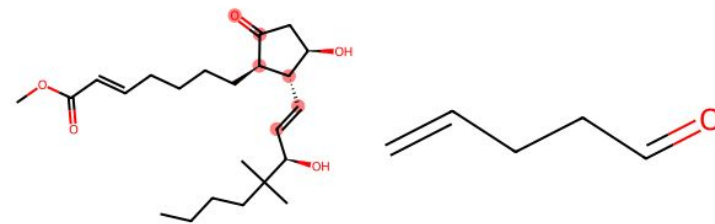
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betamethasone phosphate

['Cardiac disorders']

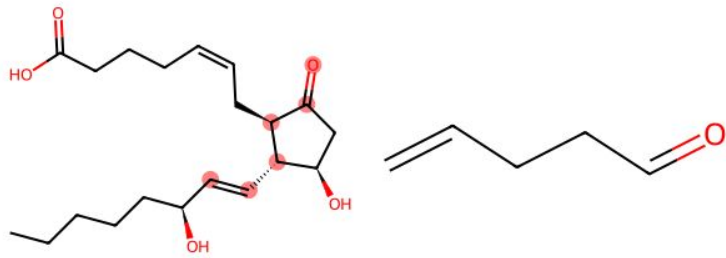
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gemeprost

['Cardiac disorders']

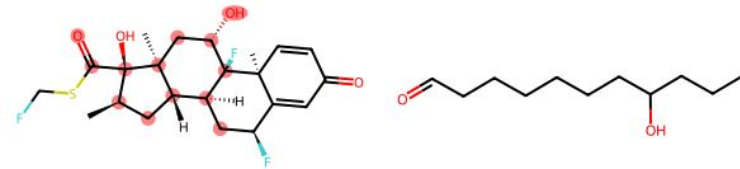
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dinoprostone

['Cardiac disorders']

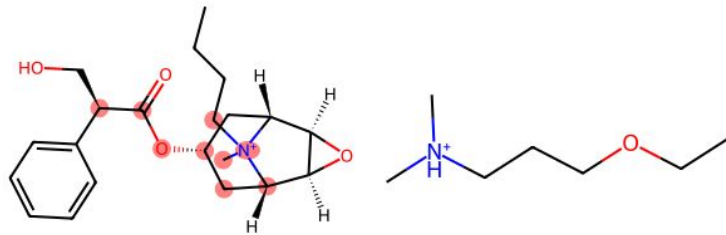
Additional Data: ['approved']



fluticasone

['Cardiac disorders']

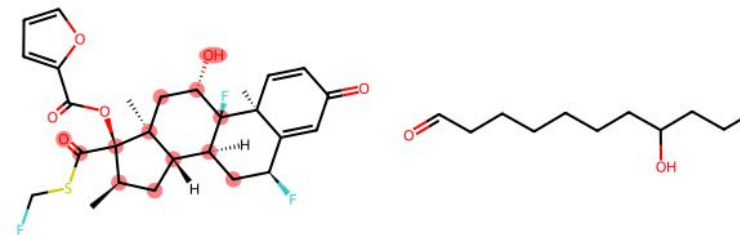
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butylscopolamine

['Cardiac disorders']

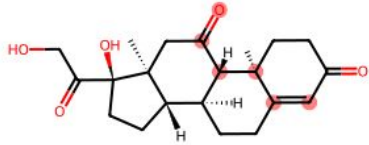
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fluticasone furoate

['Cardiac disorders']

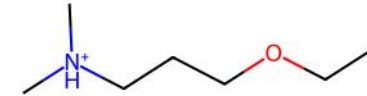
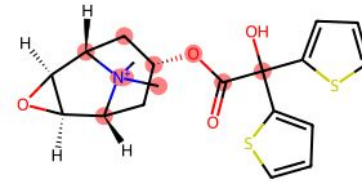
Additional Data: ['approved']



cortisone

['Cardiac disorders']

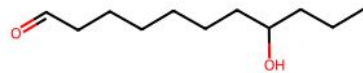
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tiotropium

['Cardiac disorders']

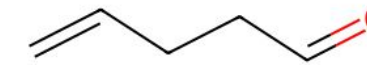
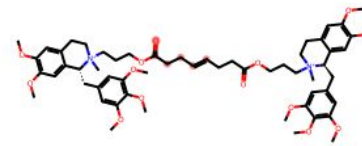
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fludrocortisone

['Cardiac disorders']

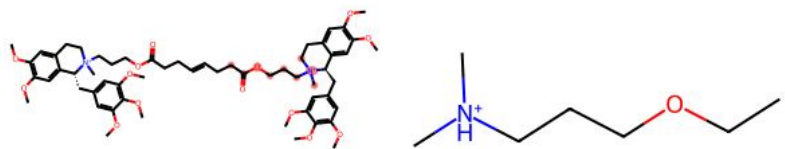
Additional Data: ['approved', 'investigational']



mivacurium

['Cardiac disorders']

Additional Data: ['approved']



mivacurium

['Cardiac disorders']

Additional Data: ['approved']

Figure S2: Hits from DrugBank compounds containing structural alerts from the top 6 presented in Figure 4(b).

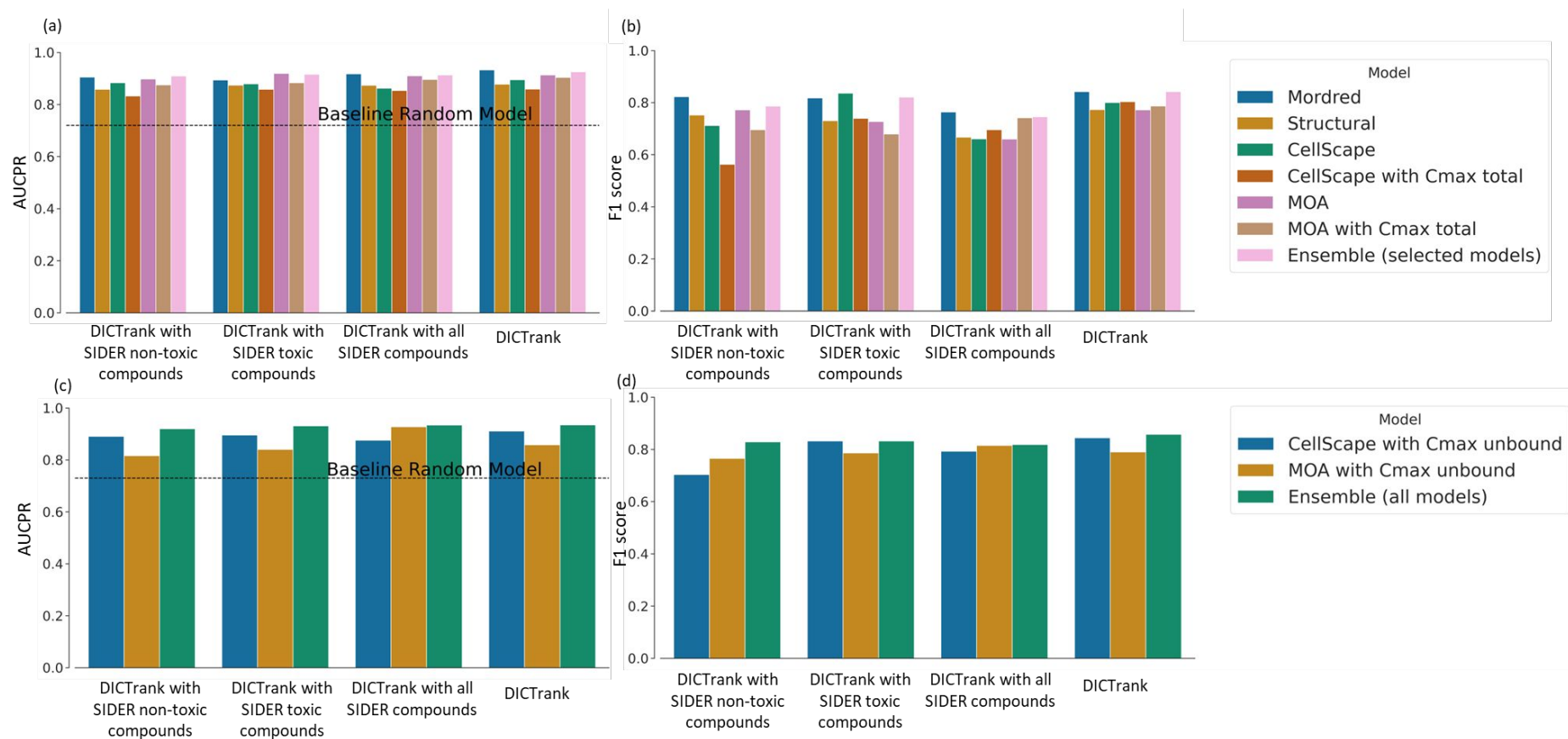


Figure S3: Evaluation metrics for models developed in this study using a larger external test set of 90 compounds evaluated using (a) AUCPR and (b) F1 scores, and for models using a subset of the external test set with 78 compounds evaluated using (c) AUCPR and (d) F1 scores

