

Selective DNA Gyrase Inhibitors: Multi-Target *In Silico* Profiling with 3D-Pharmacophores

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1. ROC plots from the GyrB ligand-based pharmacophore model validation.

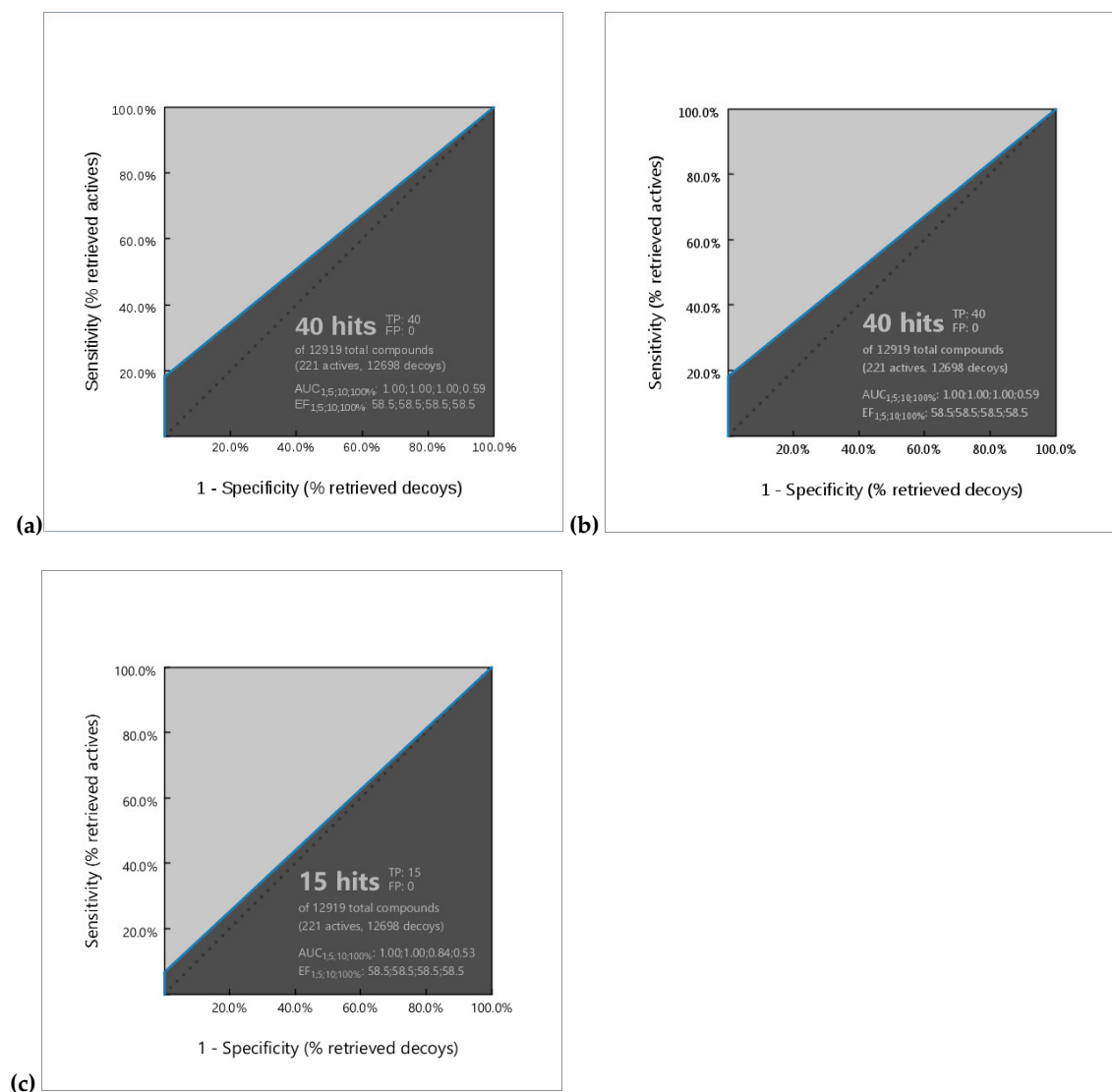


Figure S1. Validation phase of **(a) LB-GyrB-Model-5m; (b) LB-GyrB-Model-4; (c) LB-GyrB-Model-6** ligand-based pharmacophore models. Resulting ROC plot (curve shown in blue) from virtually screening 12919 compounds (221 GyrB actives and 12698 generated decoys) with the ligand-based pharmacophore model. TP = true positives; FP = false positives; AUC = area under the curve; EF = enrichment factor.

2. ROC plots from the Hsp90 ligand-based pharmacophore model validation.

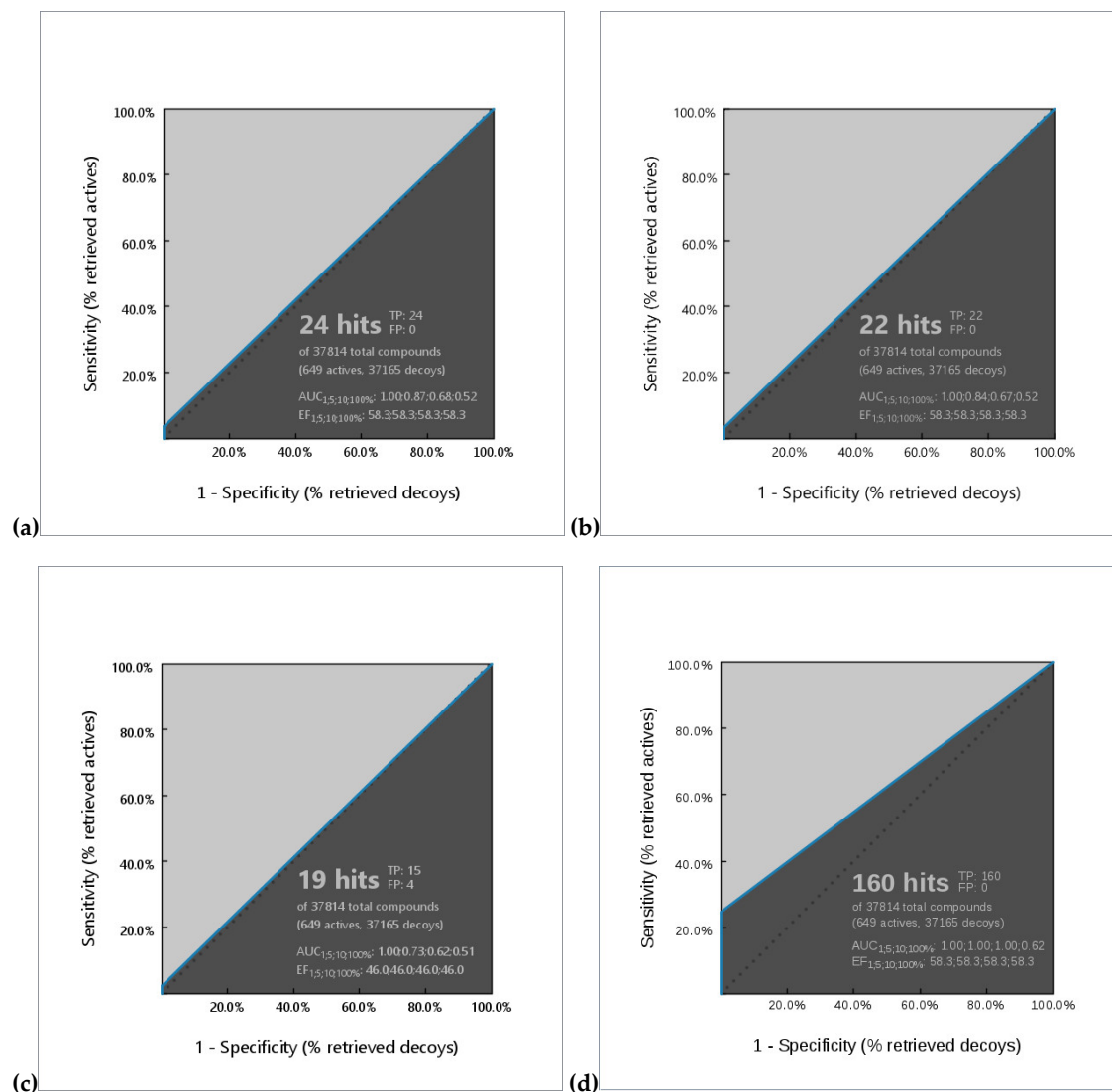


Figure S2. Validation phase of (a) LB-Hsp90-Model-3, (b) LB-Hsp90-Model-4, (c) LB-Hsp90-Model-5, and (d) LB-Hsp90-Model-6 Hsp90 ligand-based pharmacophore models. Resulting ROC plot (curve shown in blue) from virtually screening 37814 compounds (649 Hsp90 actives and 37165 generated decoys) with the ligand-based pharmacophore model. TP = true positives; FP = false positives; AUC = area under the curve; EF = enrichment factor.

3. ROC plots from the TopoII ligand-based pharmacophore model validation.

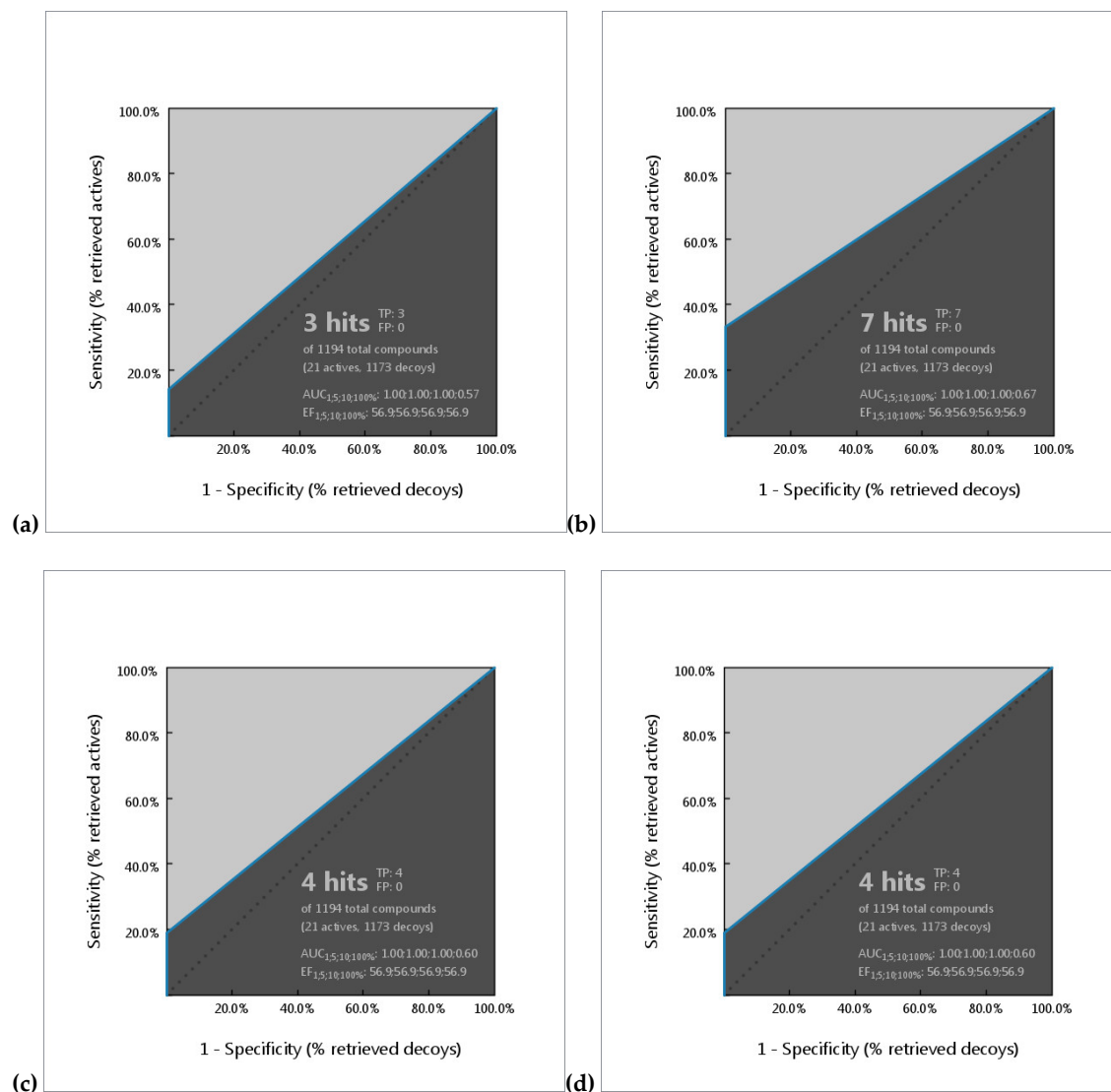


Figure S3. Validation phase of (a) **LB-TopoII-Model-1**, (b) **LB-TopoII-Model-2**, (c) **LB-TopoII-Model-3**, and (d) **LB-TopoII-Model-4** TopoII ligand-based pharmacophore models. Resulting ROC plot (curve shown in blue) from virtually screening 1194 compounds (21 TopoII actives and 1173 generated decoys) with the ligand-based pharmacophore model. TP = true positives; FP = false positives; AUC = area under the curve; EF = enrichment factor.