This document provides additional information for the article **Filtered Circular Fingerprints Improve Either Prediction Or Runtime Performance While Retaining Interpretability** submitted to the Journal of Cheminformatics by **M. Gütlein and S. Kramer** (contact: guetlein@uni-mainz.de).

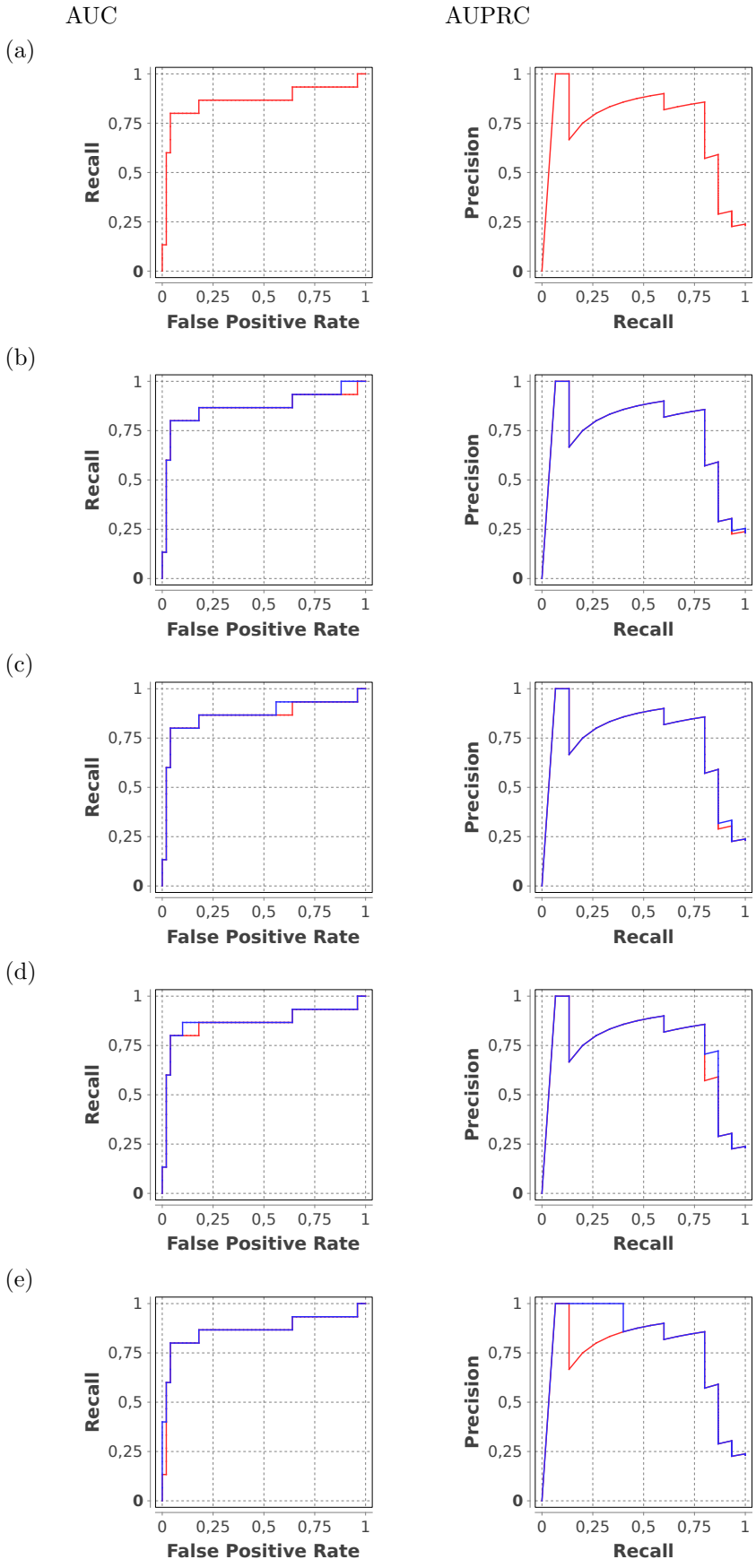
Additional file 1 — AUPRC and AUROC curves for Table 1

	Ranking of active (1) and inactive (0) compounds due to predicted probability
(a)	1101111111011100000001000000000000000000000000010000000000000000100
(b)	1101111111011100000001000000000000000000000000010000000000001000000
(c)	1101111111011100000001000000000000000000001000000000000000000000100
(d)	1101111111011100010000000000000000000000000000010000000000000000100
(e)	1111110111011100000001000000000000000000000000010000000000000000100

	AUROC	Δ	AUPRC	Δ	EF-5%	Δ	BEDROC-20	Δ	BEDROC-100	Δ
(a)	0.864		0.772		2.9		0,884		0,885	
(b)	0.869	+0.005	0.773	+0.001	2.9	0	0,889	+0,005	0,889	+0,003
(c)	0.869	+0.005	0.774	+0.002	2.9	0	0,889	+0,005	0,89	+0,004
(d)	0.869	+0.005	0.78	+0.009	2.9	0	0,89	+0,006	0,892	+0,006
(e)	0.869	+0.005	0.822	+0.051	4.3	+1.4	0,89	+0,006	0,893	+0,008

Table 1 Comparing AUPRC to other virtual screening measures when improving a reference ranking (a) at different positions (b-e).

Each bit resembles an active (1) or in-active compound (0). Each bit-string *(a-e)* corresponds to the result of a classifier that ranks all test-set compounds according to their predicted probability of being active. A perfect prediction would list all "1s" before "0s". The reference prediction *(a)* has an AUROC (the area under the ROC curve) score of 0.864 (Hence, the probability that a randomly drawn active compound is ranked higher than an in-active compound is 86.4%). We improve the reference prediction *(a)* by modifying the predicted probability of a single compound at different positions in the ranking: in *(b-d)*, a single active compound is predicted with higher probability and shifted 4 positions upwards in the ranking. In *(e)*, a single in-active compound is predicted with lower probability and is moved 4 positions downwards in the ranking. When performing virtual screening, the last change *(e)* is probably most important to us, as we are interested in the compounds that are most likely active. However, the change in AUROC is constant for *(b-e)*. EF (enrichment factor) and BEDROC (Boltzmann-Enhanced Discrimination of ROC) have the disadvantage of relying on a user defined parameter. Moreover, EF-5% changes only if the number (not the ordering) of active compounds within the top χ bits (here: 3) differs. In the contrary, AUPRC (the area under precision recall curve) has the desired property that it increases more when the affected ranking position is higher without relying on a parameter.


AUC
AUPRC
(a)
(b)
(c)
(d)
(e)
Recall
False Positive Rate
Precision
Recall
0
0,25
0,5
0,75
1