Supporting Information to

A PHYSICS-BASED SCORING APPROACH IMPROVES EARLY ENRICHMENT IN VIRTUAL SCREENING OF LARGE COMPOUND DATABASES

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PNP

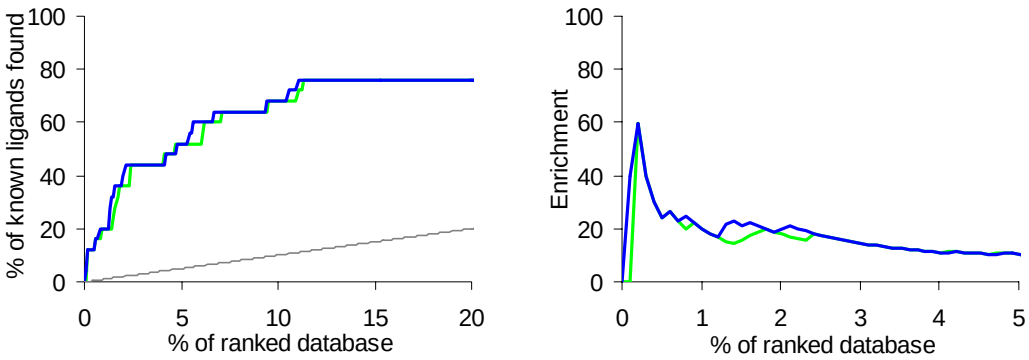
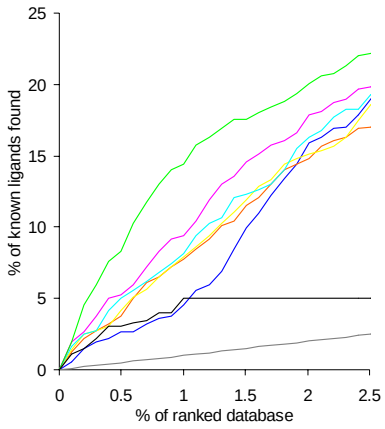
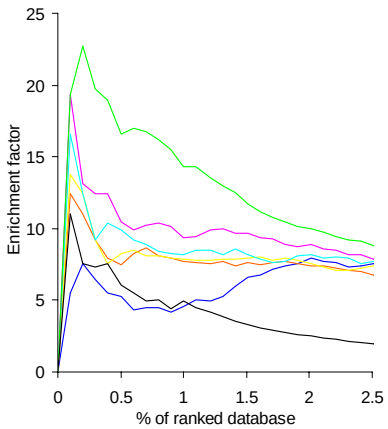


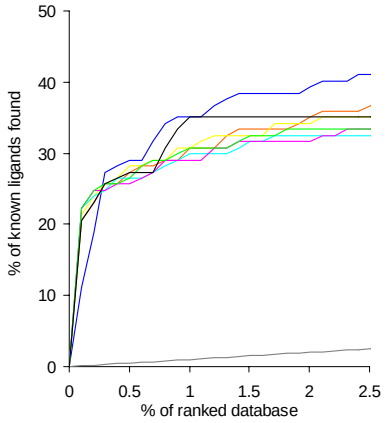
Figure S1. Enrichment plots for PNP obtained from docking with different charge states assigned to the cofactor phosphate group: $H_2PO_3^-$ (blue line) and HPO_3^{2-} (green line).

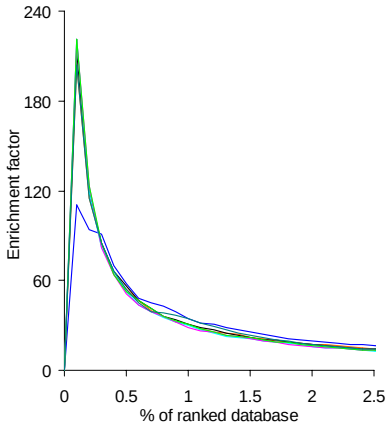
AR



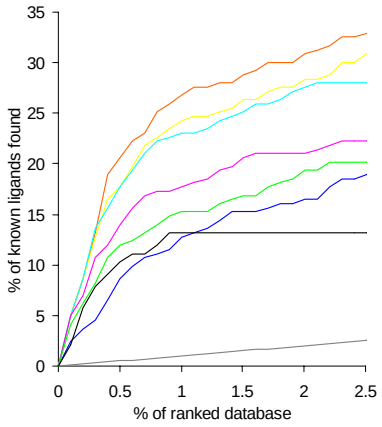


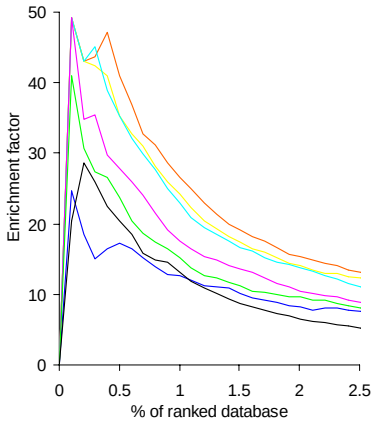
DHFR



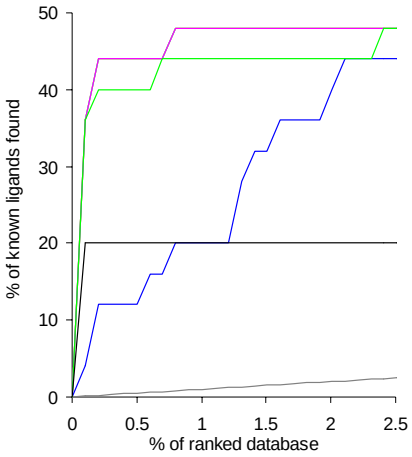


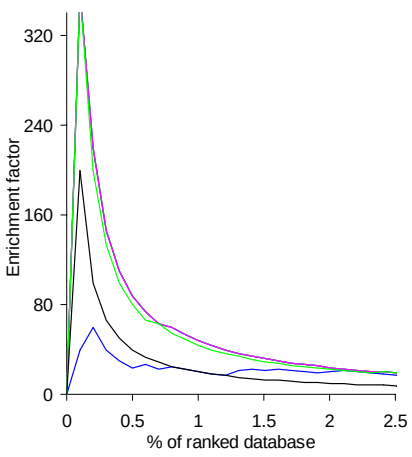
Thrombin





PNP


% of known ligands found
% of ranked database
0
10
20
30
40
50
0
0.5
1
1.5
2
2.5


Enrichment factor
% of ranked database
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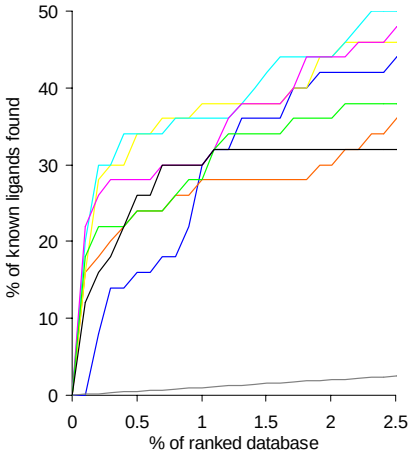
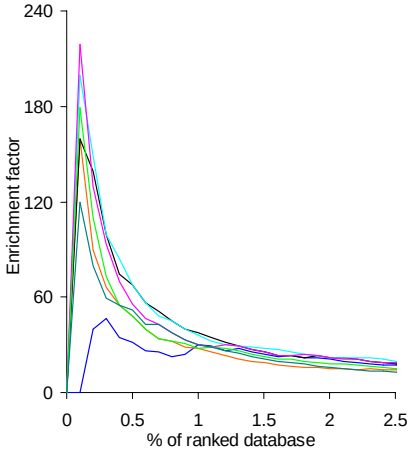
160
240
320
0
0.5
1
1.5
2
2.5

GART


% of known ligands found
% of ranked database
0
10
20
30
40
50
0
0.5
1
1.5
2
2.5


Enrichment factor
% of ranked database
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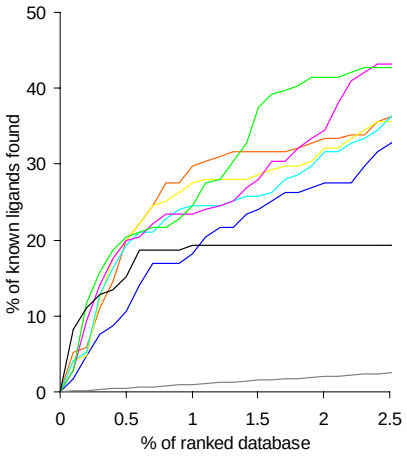
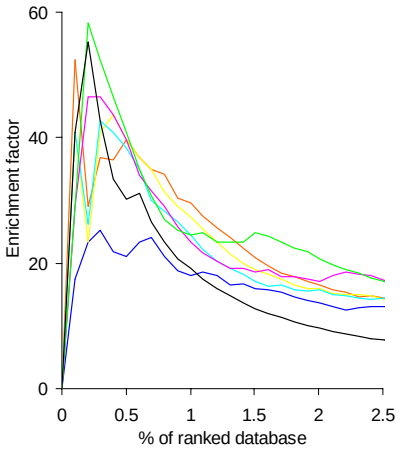
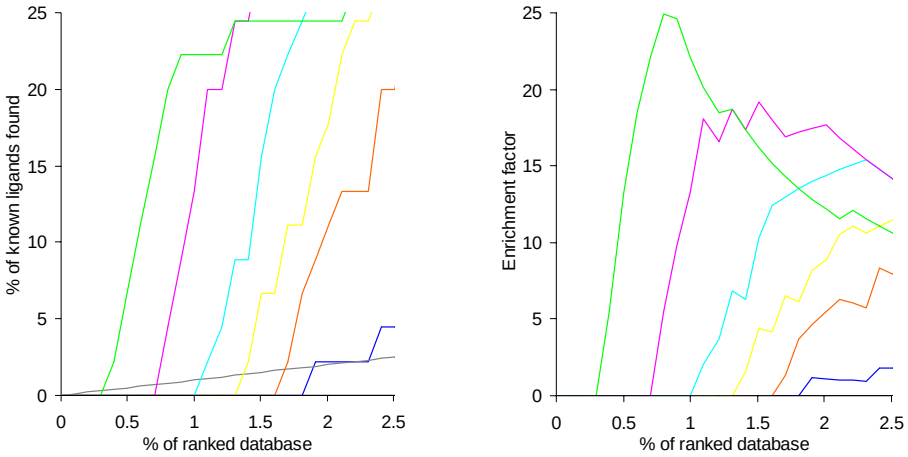
120
180
240
0
0.5
1
1.5
2
2.5

TS

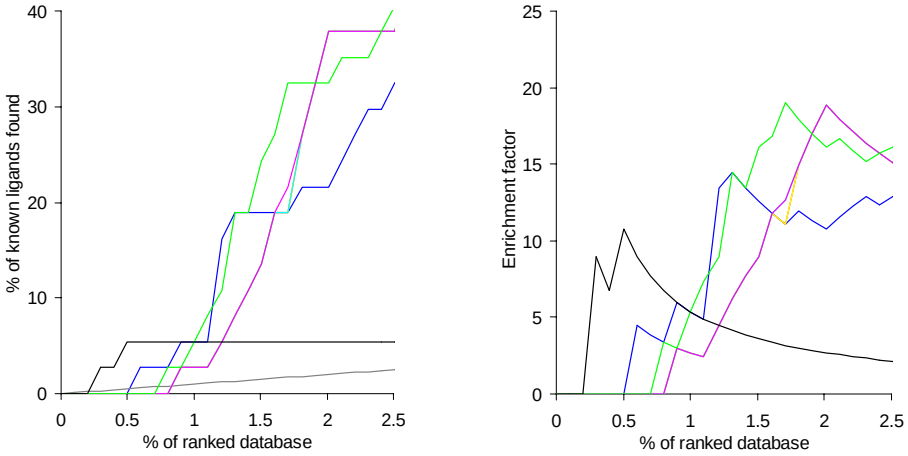

% of known ligands found
% of ranked database
0
10
20
30
40
50
0
0.5
1
1.5
2
2.5


Enrichment factor
% of ranked database
0
20
40
60
0
0.5
1
1.5
2
2.5

PARP



SAHH



AChE

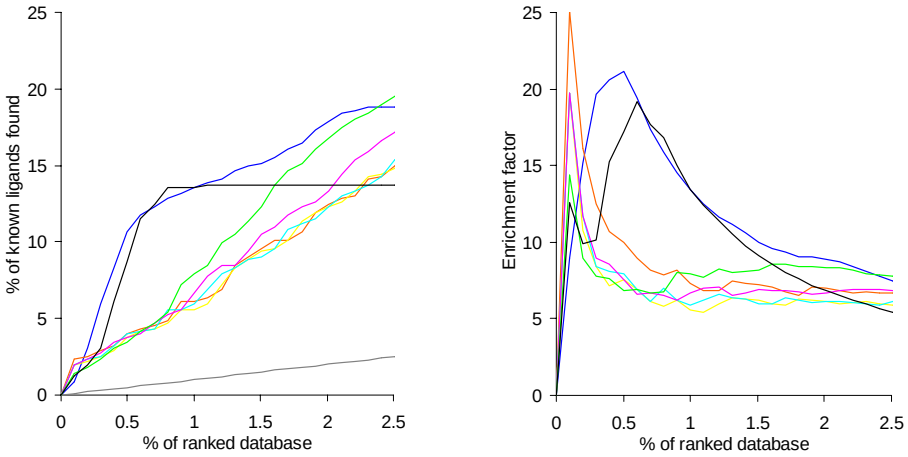


Figure S2. Enrichment plots obtained from docking (blue line), rescoring of the top 25% (orange line), the top 20% (yellow line), the top 15% (cyan line), the top 10% (purple line), the top 5% (green line) and the top 1% (black line) of the docked database.