

ROC plot validation of four crystal ligands and two leads with human MMP-1 (1HFC)

File name: /media/Seagate Backup Plus Drive/MMP-1_HUMAN/9.RESULTS/ACTIVES_AND_DECOYS_FOR_EF.maegz

Actives file: /media/Seagate Backup Plus Drive/MMP-1_HUMAN/9.RESULTS/ACTIVES_FOR_EF

Number of decoys: 1000

Enrichment Report:

Enrichment Report

Actives file: /media/Seagate Backup Plus Drive/MMP-1_HUMAN/9.RESULTS/ACTIVES_FOR_EF.maegz
 Results: /media/Seagate Backup Plus Drive/MMP-1_HUMAN/9.RESULTS/ACTIVES_AND_DECOYS_FOR_EF.maegz
 Total actives: 6
 Total ligands(aktives+decoys): 1006
 Number of ranked aktives: 6

BEDROC(alpha=160.9, alpha*Ra=0.9596): 0.836
 BEDROC(alpha=20.0, alpha*Ra=0.1193): 0.833
 BEDROC(alpha=8.0, alpha*Ra=0.0477): 0.858
 ROC: 0.96
 RIE: 15.71
 Area under accumulation curve: 0.96
 Ave. Number of outranking decoys: 39
 Minimum Tc over all active pairs: 0.021

Count and percentage of aktives in top N% of decoy results.

% Decoys	1%	2%	5%	10%	20%
# Aktives	5	5	5	5	5
% Aktives	83.3	83.3	83.3	83.3	83.3

Count and percentage of aktives in top N% of results.

% Results	1%	2%	5%	10%	20%
# Aktives	5	5	5	5	5
% Aktives	83.3	83.3	83.3	83.3	83.3

Enrichment Factors with respect to N% sample size.

% Sample	1%	2%	5%	10%	20%
EF	84	42	17	8.3	4.2
EF*	83	42	17	8.3	4.2
EF'	1.7e+02	86	34	17	8.4
DEF	76	38	15	7.5	3.8
DEF*	75	38	15	7.5	3.8
DEF'	1.5e+02	77	31	15	7.5
Eff	0.976	0.953	0.887	0.786	0.613

Enrichment Factors with respect to N% aktives recovered.

% Aktives	40%	50%	60%	70%	80%	90%	100%
EF	1.7e+02	1.7e+02	1.3e+02	1.3e+02	1.2e+02	1.2e+02	4.2
EF*	inf	inf	6.7e+02	6.7e+02	4.2e+02	4.2e+02	4.2
EF'	inf	inf	5.7e+02	5.7e+02	4.5e+02	4.5e+02	7.1
FOD	0	0	0.0003	0.0003	0.0006	0.0006	0.04

Rank	Title
1	LIGAND_2
2	LIGAND_1
3	1CGL_0ED_A_1
5	2TCL_R04
7	1HFC-PLH
242	966C-RS2

