Bayesian Interpretation of a Distance Function for Navigating High-Dimensional Descriptor Spaces

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Supplementary Figures 1 and 2

Figure 1. Comparison of DACCS and BDACCS.

Recall curves are shown for all activity classes (see Table 1 of the manuscript). Recovery rates are reported for increasingly larger numbers of ranked database compounds obtained with DACCS (black) and BDACSS (red).

Target: 5HT
Baits: 10
ADCs: 61

Target: AA2
Baits: 10
ADCs: 25

Target: ACA
Baits: 10
ADCs: 11

Target: ADR
Baits: 10
ADCs: 6

Target: ANA
Baits: 10
ADCs: 35

Target: ARI
Baits: 10
ADCs: 14

Target: ARO
Baits: 10
ADCs: 14

Target: BEN
Baits: 10
ADCs: 49

Target: CDK1
Baits: 10
ADCs: 12

Target: CDK2
Baits: 10
ADCs: 14

Target: CHO
Baits: 10
ADCs: 20

Target: COX
Baits: 10
ADCs: 21

Target: ESU
Baits: 10
ADCs: 25

Target: FAC
Baits: 10
ADCs: 4

Target: GHS
Baits: 10
ADCs: 4

Target: GLU
Baits: 10
ADCs: 4

Target: KRA
Baits: 10
ADCs: 12

Target: LAC
Baits: 10
ADCs: 19

Target: LDL
Baits: 10
ADCs: 20

Target: LIP
Baits: 10
ADCs: 31

Target: PAR
Baits: 10
ADCs: 6

Target: PDE
Baits: 10
ADCs: 11

Target: PKC
Baits: 10
ADCs: 5

Target: RTI
Baits: 10
ADCs: 5

Figure 2. Comparison of BDACCS and similarity search calculations.

Recall curves are shown for all activity classes; BDACCS (black), MACCS (red), and TGD (green). Corresponding recovery rates are reported in Table 2 of the manuscript.

Target: ANA
Baits: 10
ADCs: 35

BDACCS,log-odds — TGD,tanimoto —
MACCS,tanimoto —

Target: ARI
Baits: 10
ADCs: 14

BDACCS,log-odds — TGD,tanimoto —
MACCS,tanimoto —

Target: ARO
Baits: 10
ADCs: 14

BDACCS,log-odds — TGD,tanimoto —
MACCS,tanimoto —

Target: BEN
Baits: 10
ADCs: 49

BDACCS,log-odds — TGD,tanimoto —
MACCS,tanimoto —

Target: CDK1
Baits: 10
ADCs: 12

Target: CDK2
Baits: 10
ADCs: 14

Target: CHO
Baits: 10
ADCs: 20

Target: COX
Baits: 10
ADCs: 21

Target: D2A
Baits: 10
ADCs: 4

Target: DD1
Baits: 10
ADCs: 20

Target: DIR
Baits: 10
ADCs: 20

Target: EDN
Baits: 10
ADCs: 22

Target: GLY
Baits: 10
ADCs: 24

BDACCS,log-odds — TGD,tanimoto —
MACCS,tanimoto —

Target: GRH
Baits: 10
ADCs: 90

BDACCS,log-odds — TGD,tanimoto —
MACCS,tanimoto —

Target: H1D
Baits: 10
ADCs: 26

BDACCS,log-odds — TGD,tanimoto —
MACCS,tanimoto —

Target: H3
Baits: 10
ADCs: 42

BDACCS,log-odds — TGD,tanimoto —
MACCS,tanimoto —

Target: KRA
Baits: 10
ADCs: 12

Target: LAC
Baits: 10
ADCs: 19

Target: LDL
Baits: 10
ADCs: 20

Target: LIP
Baits: 10
ADCs: 31

Target: M2
Baits: 10
ADCs: 10

BDACCS,log-odds — TGD,tanimoto —
MACCS,tanimoto —

Target: MCH
Baits: 10
ADCs: 20

BDACCS,log-odds — TGD,tanimoto —
MACCS,tanimoto —

Target: MEL
Baits: 10
ADCs: 15

BDACCS,log-odds — TGD,tanimoto —
MACCS,tanimoto —

Target: NET
Baits: 10
ADCs: 11

BDACCS,log-odds — TGD,tanimoto —
MACCS,tanimoto —