

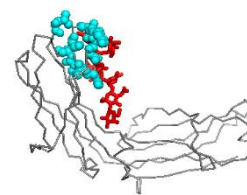
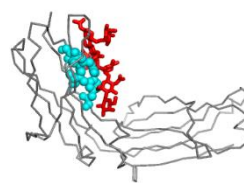
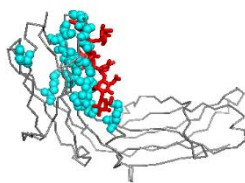
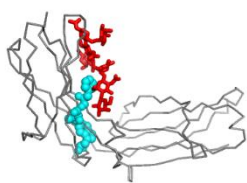
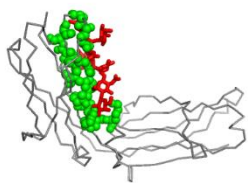
i

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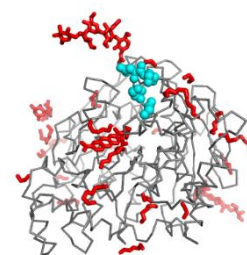
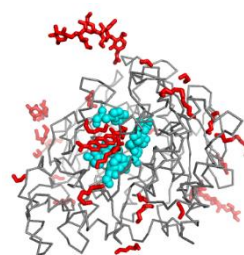
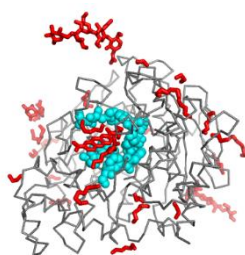
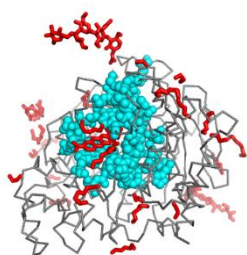
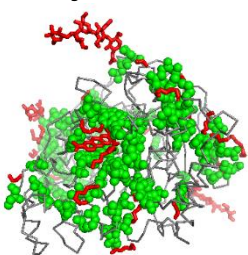
RaptorX



5djzA

BDT:0.32
MCC: 0.13BDT: **0.61**
MCC: **0.85**BDT: 0.36
MCC: 0.58
PDBhit:1h3wM(97%)BDT: 0.49
MCC: 0.55

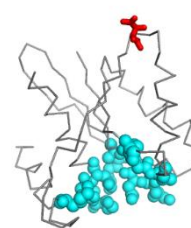
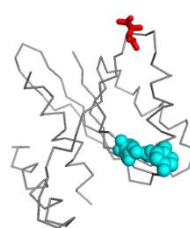
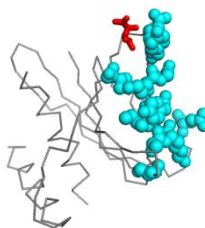
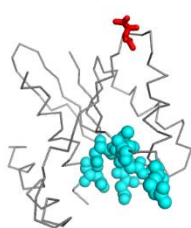
j



5e4tA

BDT: **0.34**
MCC: 0.11BDT: 0.12
MCC: **0.22**BDT: 0.1
MCC: 0.2
PDBhit:2bagA(100%)BDT:0.02
MCC: -0.03

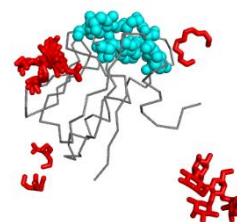
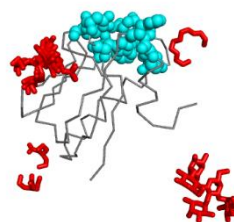
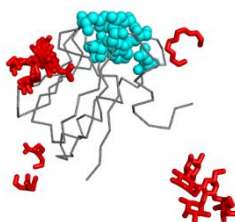
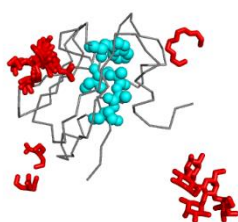
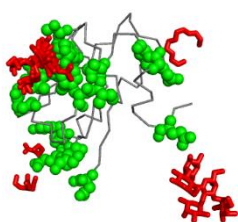
k



5e6fB

BDT:0.05
MCC: -0.02BDT: **0.32**
MCC: **0.41**BDT:0.06
MCC: -0.02
PDBhit:3ezwA (10%)BDT:0.04
MCC: -0.04

l



5elfJ

BDT: 0.08
MCC: -0.11BDT:0.1
MCC: -0.13BDT: 0.19
MCC: -0.06
PDBhit:1pziF(81%)BDT:0.16
MCC: -0.05

S1 Fig

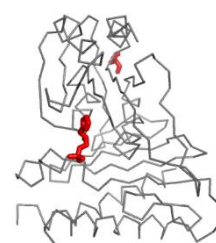
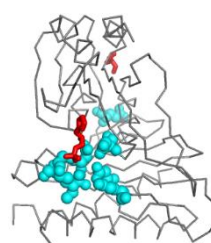
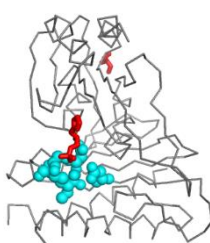
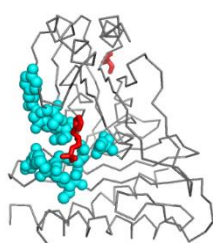
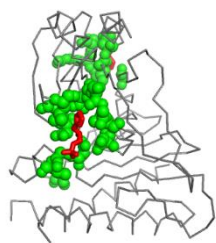
m

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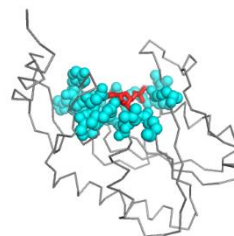
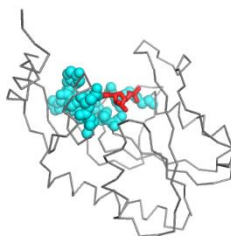
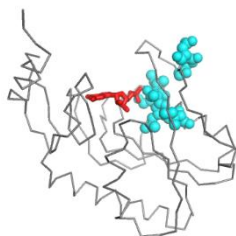
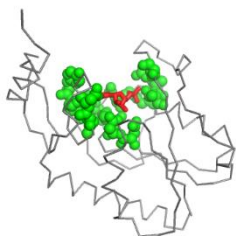
RaptorX



5eq9D

BDT: **0.56**
MCC: 0.2BDT: 0.27
MCC: 0.29BDT: 0.29
MCC: **0.33**
PDBhit:1nv6A(17%)BDT: 0
MCC: 0

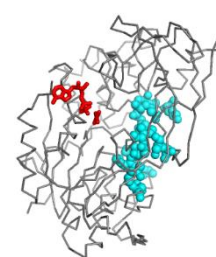
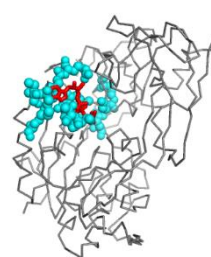
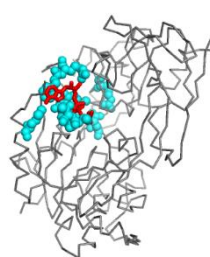
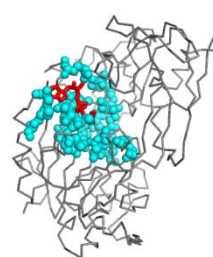
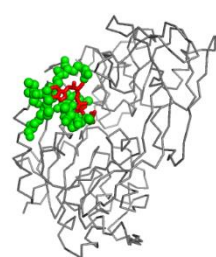
n



5esxB

BDT: 0.44
MCC: 0.4BDT: 0.61
MCC: 0.66BDT: **0.8**
MCC: **0.69**
PDBhit:4racA(25%)BDT: 0
MCC: 0

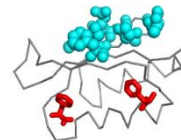
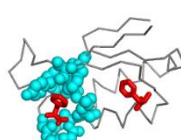
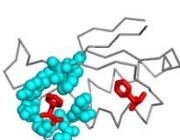
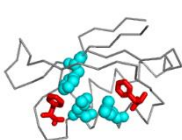
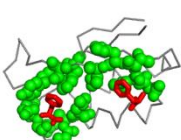
o



5fhfA

BDT: 0.55
MCC: 0.53BDT: 0.8
MCC: 0.74BDT: **0.86**
MCC: **0.89**
PDBhit:5ftbA(99%)BDT: 0.08
MCC: -0.03

p



5fiiD

BDT:0.16
MCC: 0.25BDT :0.6
MCC: **0.76**BDT: **0.62**
MCC:0.59
PDBhit: 3mwbB(12%)BDT:0.17
MCC: -0.15

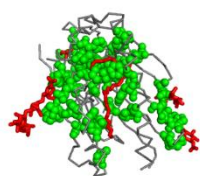
q

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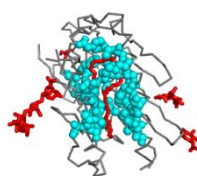
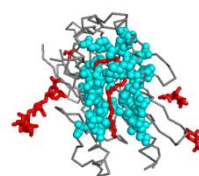
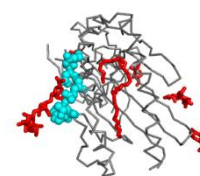
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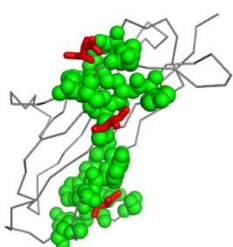
RaptorX



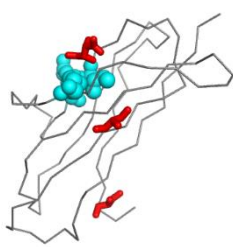
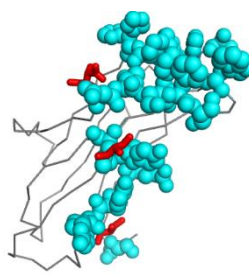
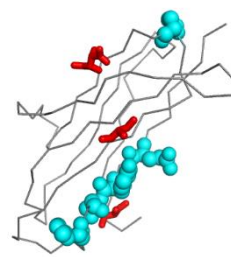
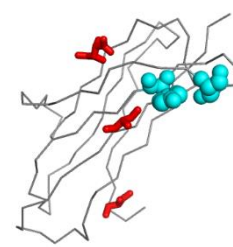
5fkpA

BDT:0.14
MCC: -0.03BDT:0.38
MCC:0.29BDT:0.43
MCC:0.34
PDBhit:4y16A(99%)BDT:0.3
MCC:0.29

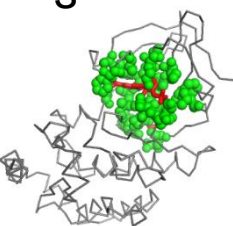
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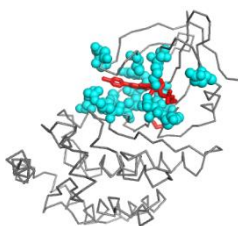
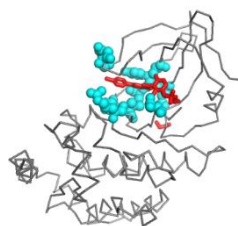
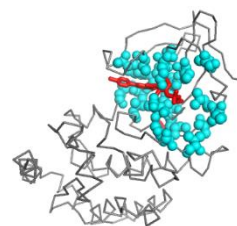
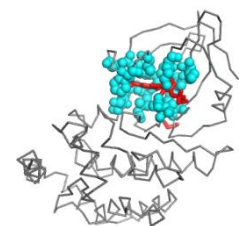
5fkpB

BDT:0.16
MCC:0.24BDT:0.55
MCC:0.05BDT:0.2
MCC:0.14
PDBhit:4ra3C(69%)BDT:0.1
MCC:0.22

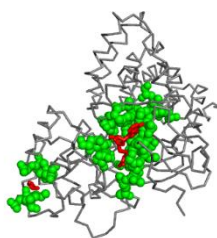
s



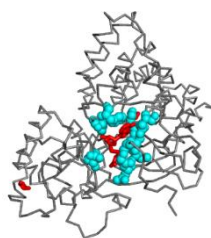
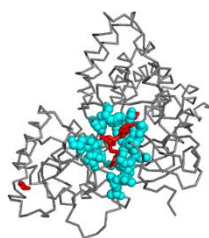
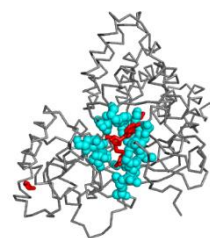
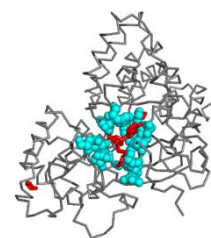
5hesB

BDT:0.76
MCC:0.51BDT:0.34
MCC:0.34BDT:0.81
MCC:0.65
PDBhit: 5e8yA (30%)BDT:0.70
MCC:0.70

t



5hq8B

BDT:0.62
MCC:0.49BDT:0.5
MCC:0.69BDT:0.48
MCC:0.68
PDBhit:3pdnA(99%)BDT:0.42
MCC:0.63

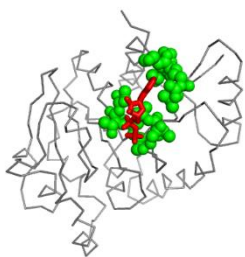
U

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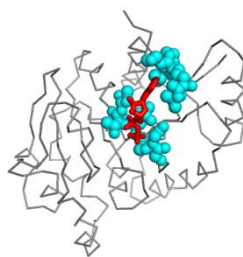
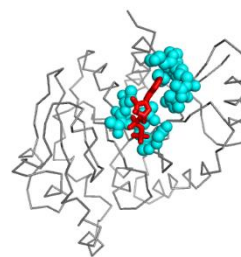
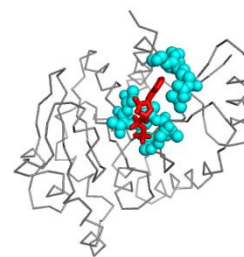
COFACTOR

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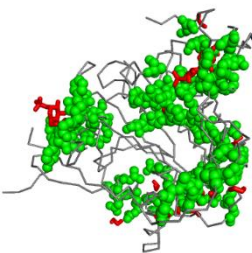
RaptorX



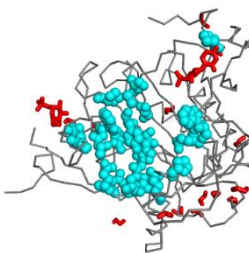
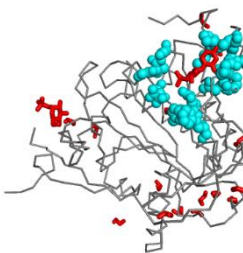
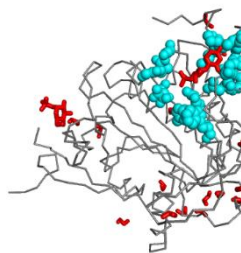
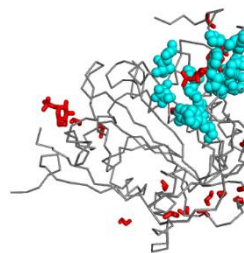
5ihpB

MCC:0.5
BDT:0.5BDT:0.88
MCC:0.74BDT:0.97
MCC:0.91
PDBhit:1ionA(31%)BDT:0.91
MCC:0.95

V



5in3B

BDT:0.1
MCC: -0.02BDT:0.14
MCC:0.2BDT:0.18
MCC:0.29
PDBhit:1guqC(56%)BDT :0.25
MCC:0.39