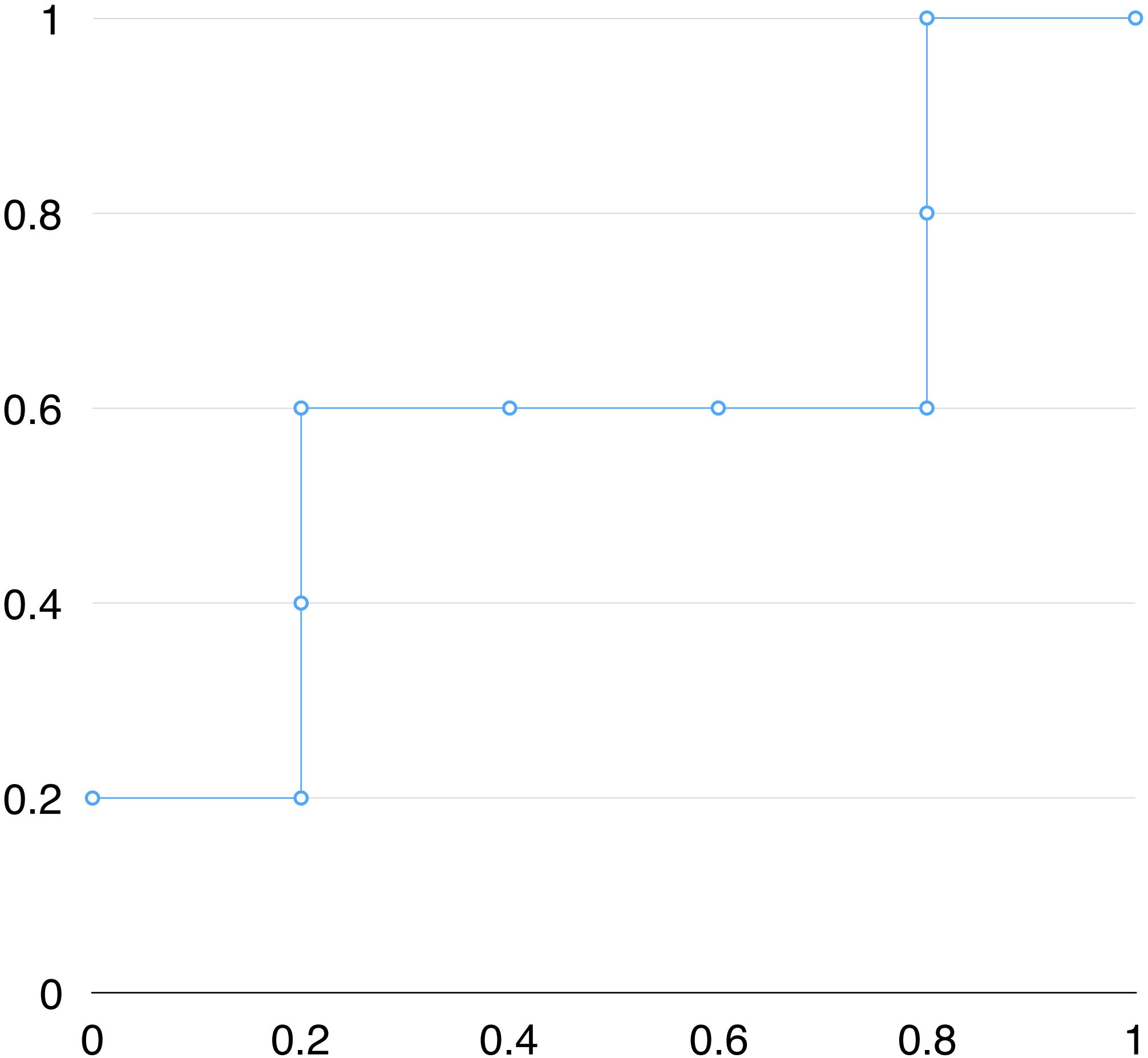
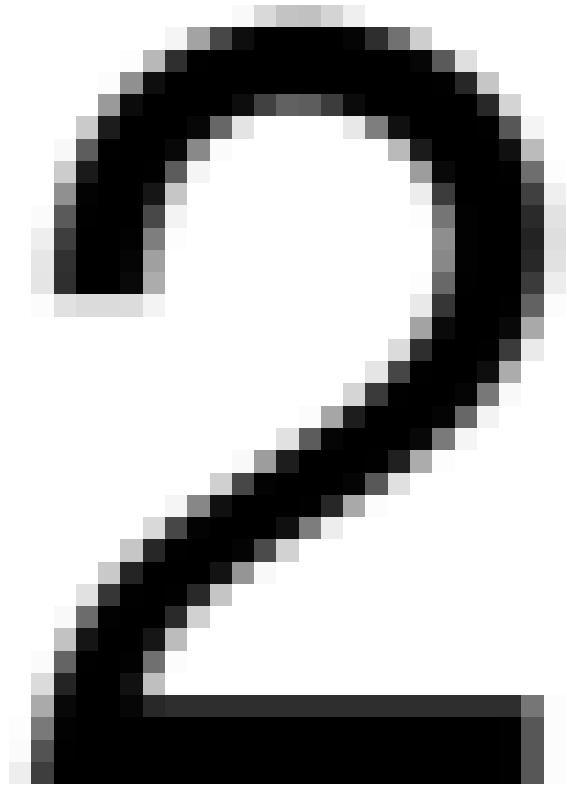
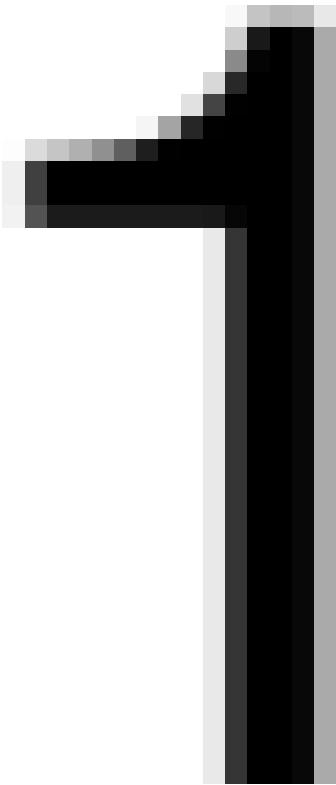


Operating Characteristic (ROC) Curve

score	fraction of actives	fraction of inactives
-53.4	0.2	0
-50.2	0.2	0.2
-49.2	0.4	0.2
-45.7	0.6	0.2
-42.1	0.6	0.4
-35.2	0.6	0.6
-30.0	0.6	0.8
-21.3	0.8	0.8
-20.7	1.0	0.8
-4.2	1.0	1.0

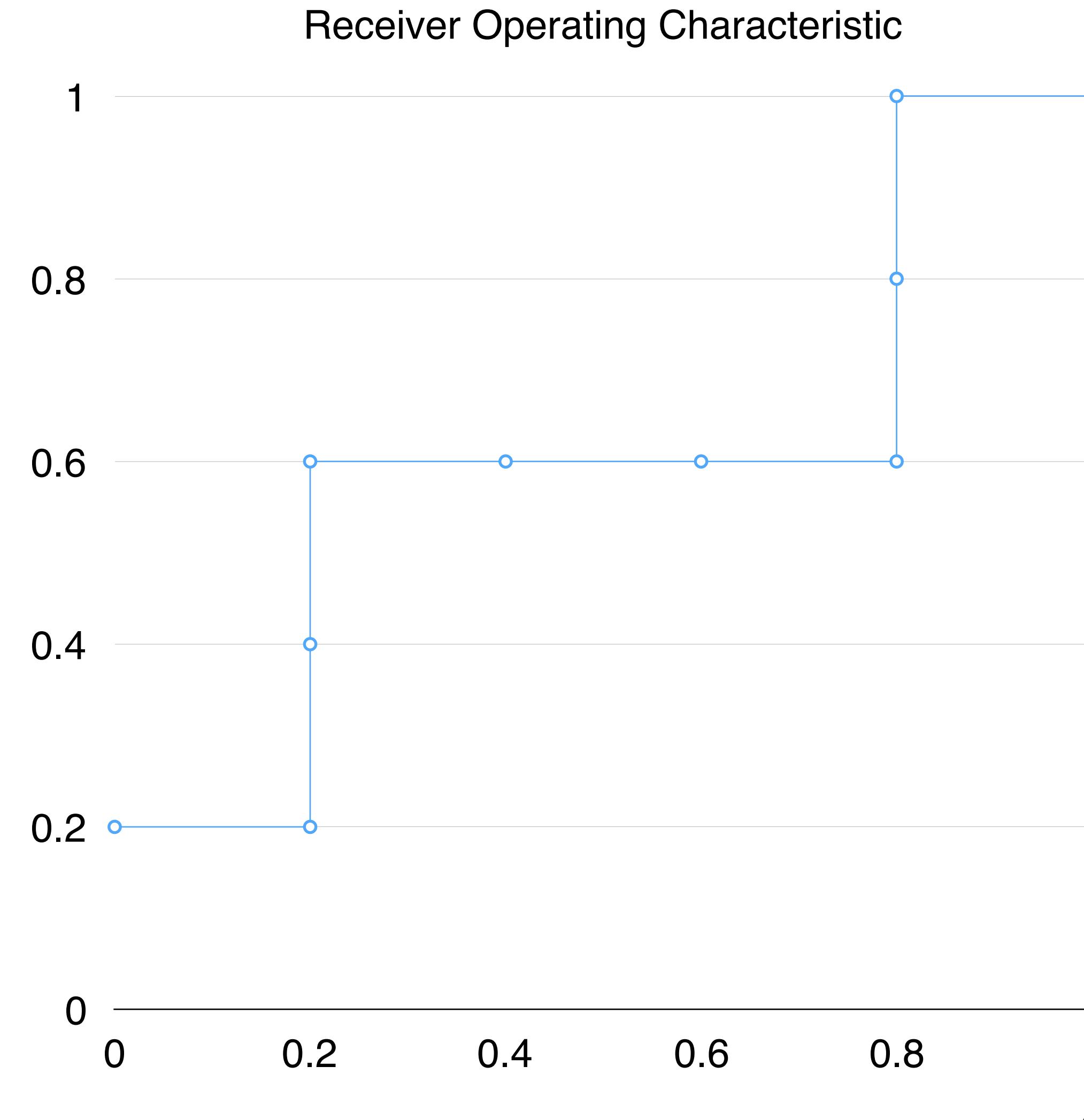
Receiver Operating Characteristic



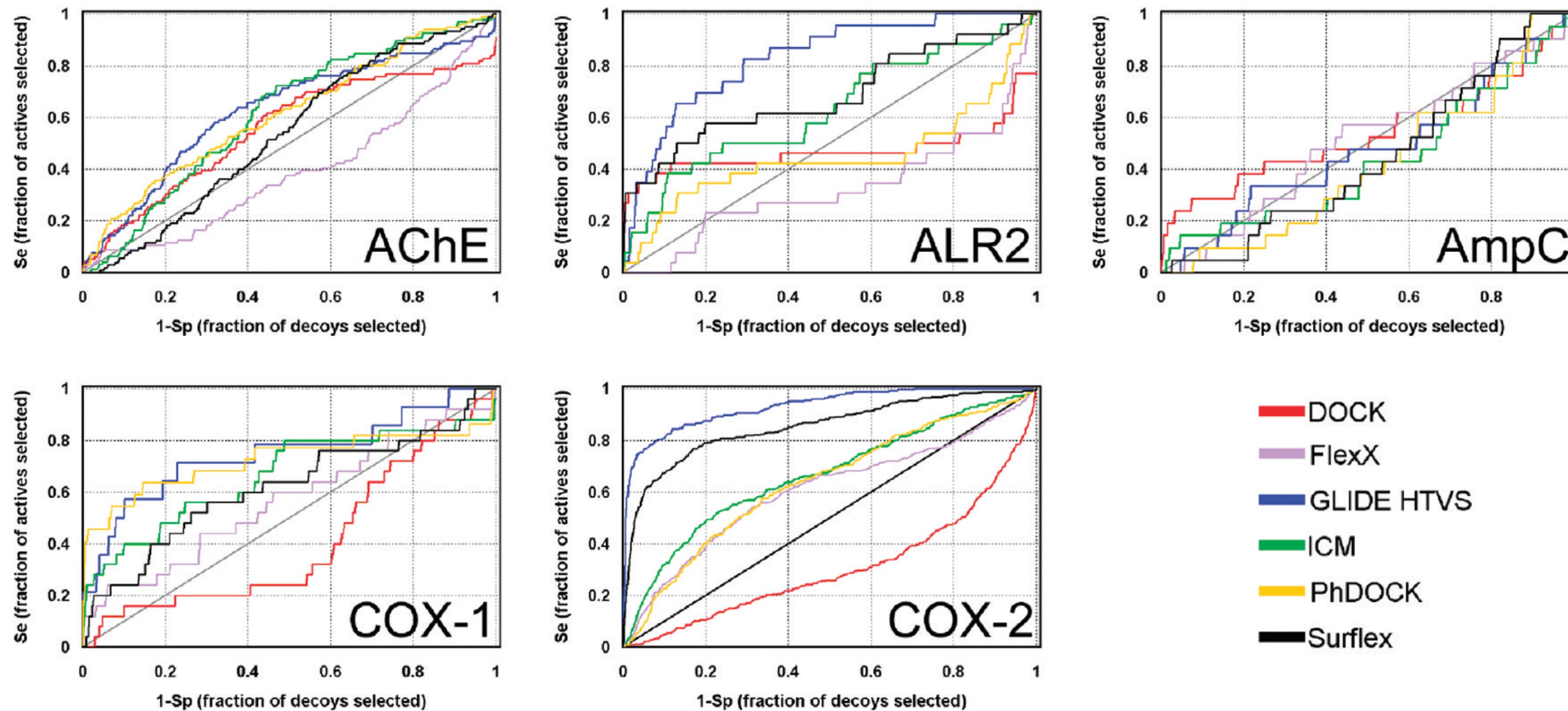


The Receiver Operating Characteristic (ROC) Curve

score	fraction of actives	fraction of inactives
-53.4	0.2	0
-50.2	0.2	0.2
-49.2	0.4	0.2
-45.7	0.6	0.2
-42.1	0.6	0.4
-35.2	0.6	0.6
-30.0	0.6	0.8
-21.3	0.8	0.8
-20.7	1.0	0.8
-4.2	1.0	1.0



Molecular docking is often an unreliable binary classifier



Cross et al, 2009