



ROCS Statistics*	Cluster 1 Actives (7)	FXa DUD Actives (792)
<b>AUC</b>	0.999847	0.743565
95% confidence min	0.999499	0.724189
95% confidence max	1.000000	0.761754
<b>0.5% Enrichment</b>	200.000000	30.000189
95% confidence min	200.000000	25.345045
95% confidence max	200.000015	35.400517
<b>1.0% Enrichment</b>	100.000000	19.191874
95% confidence min	100.000000	16.416040
95% confidence max	100.000008	21.774193
<b>2.0% Enrichment</b>	50.000000	12.311981
95% confidence min	50.000000	10.945273
95% confidence max	50.000004	14.037267

\* Based on Tanimoto Combo Score

ROCS Statistics*	Cluster 2 Actives (8)	FXa DUD Actives (792)
<b>AUC</b>	0.999847	0.709970
95% confidence min	0.999499	0.688660
95% confidence max	1.000000	0.730982
<b>0.5% Enrichment</b>	200.000000	31.396284
95% confidence min	200.000000	26.294821
95% confidence max	200.000015	36.251541
<b>1.0% Enrichment</b>	100.000000	18.228065
95% confidence min	100.000000	15.374842
95% confidence max	100.000008	20.838795
<b>2.0% Enrichment</b>	50.000000	12.393811
95% confidence min	50.000000	10.704787
95% confidence max	50.000004	13.928113

\* Based on Tanimoto Combo Score

ROCS Statistics*	Cluster 3 Actives (5)	FXa DUD Actives (792)
<b>AUC</b>	0.994793	0.790717
95% confidence min	0.999041	0.772904
95% confidence max	1.000000	0.808000
<b>0.5% Enrichment</b>	198.666672	51.408276
95% confidence min	200.000000	44.923859
95% confidence max	200.000015	57.985264
<b>1.0% Enrichment</b>	99.333336	31.495468
95% confidence min	100.000000	28.328981
95% confidence max	100.000008	34.753662
<b>2.0% Enrichment</b>	49.666668	17.344225
95% confidence min	50.000000	15.571775
95% confidence max	50.000004	18.918919

\* Based on Tanimoto Combo Score

**Supplementary Figure 1.** ROCS shape-based query validation statistics for Cluster 1 (A), Cluster 2 (B) and Cluster 3 (C), using the active molecules for each cluster or all available FXa ligand from the DUD-E database