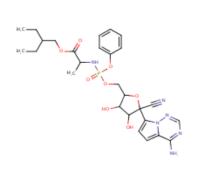
Library screened ChEMBL

Screening method Electroshape

Date Thu Jan 2 11:13:06 2020

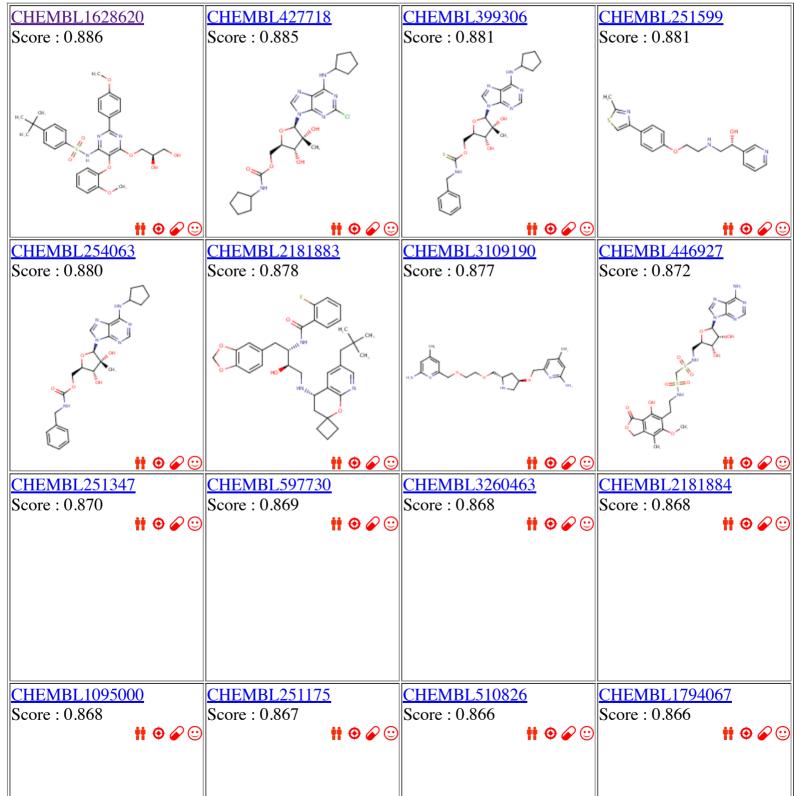
If you publish these results, please, cite the following paper: <u>Zoete, V., Daina, A., Bovigny, C., & Michielin, O. SwissSimilarity: A Web Tool for Low to Ultra High Throughput Ligand-Based Virtual Screening., *J. Chem. Inf. Model.*, **2016**, *56*(8), 1399-1404.</u>





Results









	<u>CHEMBL2064652</u> Score : 0.849 †† ⊕ ଢ ©	CHEMBL359519 Score: 0.848	CHEMBL240716 Score: 0.848 # ♥ ♥ □
	CHEMBL2165028 Score : 0.848	CHEMBL2064656 Score: 0.848	CHEMBL205043 Score: 0.848 ## ♥ № ©
CHEMBL 200072 Score: 0.848	CHEMBL1915981 Score: 0.848	CHEMBL1770706 Score: 0.848	CHEMBL358924 Score: 0.847
II I	CHEMBL212870 Score: 0.847	CHEMBL206941 Score: 0.847	CHEMBL369773 Score: 0.846
	CHEMBL200279 Score: 0.846	CHEMBL1801416 Score: 0.846	CHEMBL1774349 Score: 0.846 ##





II I	CHEMBL181819 Score: 0.839	CHEMBL1084145 Score: 0.839	CHEMBL610235 Score: 0.838
	CHEMBL439335 Score: 0.838	CHEMBL381917 Score: 0.838	CHEMBL374364 Score: 0.838
CHEMBL258421 Score: 0.838	CHEMBL211578 Score : 0.838	CHEMBL1089387 Score: 0.838	CHEMBL402574 Score: 0.837
CHEMBL334221 Score: 0.837	CHEMBL3215627 Score : 0.837	CHEMBL303342 Score: 0.837	CHEMBL2402024 Score: 0.837
II I	CHEMBL211841 Score : 0.837	CHEMBL2064640 Score : 0.837	CHEMBL206085 Score: 0.837

CHEMBL500157	CHEMBL328917	CHEMBL3217167	CHEMBL3121114
			Score: 0.836
# ⊕ 6 ⊕	# ⊕ 6 ⊙	# ⊕ 6 ⊕	# ⊕ 6 9
		II 🗸 🗸	
	<u>CHEMBL237381</u>	<u>CHEMBL2349327</u>	<u>CHEMBL221751</u>
II II			Score : 0.836
# ⊕ 🔗 😊	†† ⊕ 🔗 😉	# ⊕ 	†† ⊕
CHEMBL2089342	<u>CHEMBL182344</u>	CHEMBL1822642	CHEMBL477667
			Score: 0.835
# 6 ©	# * * * *	# ⊕ 6 ⊕	# 6 ©
	🗘 🗸	🗸 🗸	
CHEMPI 420701	CHEMPI 402977	CHEMBI 2260760	CHEMBI 202505
	<u>CHEMBL403877</u> Score: 0.835		<u>CHEMBL303595</u> Score: 0.835
Score : 0.835 # ⊕ 6 9	score: 0.855 # ⊕ 6 ⊙	Score : 0.835 # ⊕ 6 ⊕	# ⊕ 6 9
II • • •	11 🗣 🌽 🥥	11 4 6	11 4 6
			<u>CHEMBL182841</u>
			Score: 0.835
# ⊕ 🔗 🙂	# ⊕ 	# ⊕ 🔗 ⊙	ii ⊕ 🔗 😉



CHEMBL200854 Score: 0.833	<u>CHEMBL1915978</u> Score : 0.833 *** 	<u>CHEMBL552269</u> Score : 0.832 †† 	<u>CHEMBL502985</u> Score : 0.832
CHEMBL501242 Score : 0.832	CHEMBL487247 Score : 0.832 ## � 6 ©	CHEMBL436649 Score : 0.832	CHEMBL252960 Score : 0.832
CHEMBL252755 Score: 0.832	CHEMBL235695 Score : 0.832		CHEMBL2064637 Score: 0.832
CHEMBL2048211 Score: 0.832	CHEMBL204781 Score: 0.832	CHEMBL184407 Score: 0.832	CHEMBL181905 Score: 0.832
CHEMBL1083923 Score: 0.832	CHEMBL78357 Score : 0.831	CHEMBL491616 Score : 0.831	CHEMBL477666 Score: 0.831

CHEMDI 464024	CUEMDI 460071	CHEMBI 2027012	CHEMBI 201421
<u>CHEMBL464924</u>	1	<u>CHEMBL3037912</u>	<u>CHEMBL291421</u>
			Score: 0.831
†† ⊕ 🔗 😉	†† ⊕ 🔗 🙂	†† ⊕ 	†† ⊕ 🔗 😉
CHEMDI 257405	CHEMPI 2414526	CHEMDI 219119	CHEMPI 2064645
<u>CHEMBL257405</u>		<u>CHEMBL218118</u>	<u>CHEMBL2064645</u>
Score: 0.831		Score: 0.831	Score: 0.831
†† ⊕ 🔗 🙂	†† ⊕ 🔗 🙂	†† 🏵 🔗 😉	†† ⊕ 🔗 🙂
CHEN IDI 2000 ACA1	CHENTEL 207700	CHENTEL 100504	CHEN (DI 1005101
<u>CHEMBL2064641</u>	I I	<u>CHEMBL182534</u>	<u>CHEMBL1825131</u>
		Score: 0.831	Score: 0.831
†† ⊕ 🔗 😉	†† ⊕ 	†† ⊕ 🔗 ⊙	†† ⊕ 🔗 😉
CYYPY (DY (OQ 100	CYYPY FDY FOOT CC	CYYPY FDY FOA CCF	CYYPY CDY CORE 44
CHEMBL603422	<u>CHEMBL599566</u>	<u>CHEMBL521665</u>	<u>CHEMBL507541</u>
Score: 0.830	Score: 0.830	Score: 0.830	Score: 0.830
†† ⊕ 	# ⊕ 	# 😌 🔗 😉	# ⊕
CHEMBL453211	CHEMBL448015	CHEMBL399522	CHEMBL393791
Score: 0.830		Score: 0.830	Score: 0.830
	I I		
# ⊕ ⊘ ⊙	# ⊕ 	# ⊕ 🎤 😊	# ⊕
CHEMDI 24107/0	CHEMDI 222945	CHEMDI 2191929	CHEMPI 2152201
<u>CHEMBL2419769</u>	<u>CHEMBL223845</u>	<u>CHEMBL2181829</u>	<u>CHEMBL2153391</u>



	CHEMBL2407491 Score: 0.828		CHEMBL233059 Score: 0.828
	<u>CHEMBL222198</u> Score : 0.828 *† 		CHEMBL204520 Score : 0.828
	CHEMBL1801050 Score: 0.828 ## �		CHEMBL596904 Score: 0.827
II II	CHEMBL515442 Score: 0.827		CHEMBL510557 Score: 0.827
	CHEMBL396043 Score : 0.827	CHEMBL371022 Score: 0.827	CHEMBL231620 Score : 0.827





CHEMBL3092943 Score: 0.825	CHEMBL27376 Score: 0.825	CHEMBL272828 Score: 0.825
CHEMBL2048207 Score: 0.825		CHEMBL1822643 Score: 0.825
CHEMBL1779404 Score: 0.825	CHEMBL1084667 Score: 0.825	CHEMBL599387 Score: 0.824
CHEMBL504917 Score : 0.824	CHEMBL471153 Score : 0.824	CHEMBL399839 Score: 0.824
CHEMBL3215851 Score : 0.824 ##	CHEMBL318777 Score: 0.824	CHEMBL3088174 Score: 0.824

CHEMBL307172	CHEMBL261188	CHEMBL2181881	CHEMBL2171439
			Score: 0.824
†† ⊕ 	I I	## 🕹 🏈 😉	# � � ⊙
<u>CHEMBL2113428</u>			<u>CHEMBL183713</u>
			Score: 0.824
†† ⊕ 	†† ⊕ 	†† ⊕ 🔗 😉	†† ⊕ 🔗 😉
CHEMPI 1922654	CHEMBI 1000114	CHEMDI 602970	CHEMPI 512060
CHEMBL1822654 Score: 0.824		<u> </u>	CHEMBL513069
Score : 0.824 # ⊕ 6 ⊙	I I	Score : 0.823 # ⊕ 6 9 9	Score : 0.823 # ⊕ ? • •
H & & &	†† ⊕ 	11 4 6 9	11 4 2 9
CHEMBL513048	CHEMBL510885	CHEMBL399840	CHEMBL385698
Score: 0.823			Score: 0.823
†† ⊕ 	# ⊕ 	# 0 🔗 😊	# ⊕
<u>CHEMBL367133</u>		<u>CHEMBL3264923</u>	<u>CHEMBL3235991</u>
Score: 0.823		Score: 0.823	Score: 0.823
# ⊕ 	†† ⊕ 	†† ⊕ 🔗 😉	†† ⊕
CHEMPI 245192	CHEMPI 2240221	CHEMPI 2240210	CHEMPI 222260
CHEMBL245182	CHEMBL2349331	<u>CHEMBL2349319</u>	<u>CHEMBL233260</u>
Score: 0.823	I I	Score: 0.823	Score: 0.823



