Enchanting molecules

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November 25, 2022

Abstract. We suggest the use of the molecules (7a'R,8'R)-2'-fluoro-N-methyl-2',3',7',7a',8',9',11',11a'-octahydro-1'H-spiro[oxetane-3,10'-pyrido[3,2,1-de]phenazin]-8'-amine,3-fluoro-N-((S)-1,1,1-trifluoropropan-2-yl)-1,2,3,4-tetrahydroquinolin-8-amine, (2S)-2-((3-fluoro-1,2,3,4-tetrahydroquinolin-8-yl)amino)cyclohexanol and N-butyl-3-fluoro-1,2,3,4-tetrahydroquinolin-8-amine for the fight against numerous diseases, after *in silico* analysis.

Keywords: chemoinformatic and drug discovery.

"Jesus said unto her, I am the resurrection, and the life: he that believeth in me, though he were dead, yet shall he live:" — John 11:25 (KJV)

1. Introduction

In this paper, we suggest using the molecules below [Figures 1, 2, 3 and 4] to combat countless diseases.

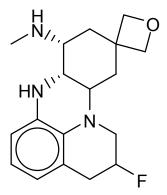


Fig.1. The molecule 1: (7a'R,8'R)-2'-fluoro-N-methyl-2',3',7',7a',8',9',11',11a'-octahydro-1'H-spiro[oxetane-3,10'-pyrido[3,2,1-de]phenazin]-8'-amine (C₁₈H₂₄FN₃O).

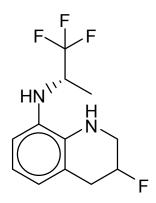


Fig. 2. The molecule 2: 3-fluoro-N-((S)-1,1,1-trifluoropropan-2-yl)-1,2,3,4-tetrahydroquinolin-8-amine (C₁₂H₁₄F₄N₂).

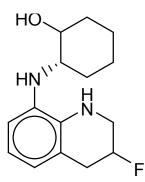


Fig. 3. The molecule 3: (2S)-2-((3-fluoro-1,2,3,4-tetrahydroquinolin-8-yl)amino)cyclohexanol (C₁₅H₂₁FN₂O).

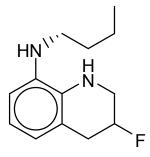


Fig. 4. The molecule 4: N-butyl-3-fluoro-1,2,3,4-tetrahydroquinolin-8-amine (C₁₃H₁₉FN₂).

While reading this article, we will show some physicochemical descriptors as well as to predict ADME parameters, pharmacokinetic properties, druglike nature and medicinal chemistry friendliness of the molecule in question, with the help of the SwissADME website, see (Daina et al., 2017),(Daina et al., 2014) and (Daina and Zoete, 2016).Next, we will show the probabilities of the indications of predicted targets, with the help of the Super-PRED (Nickel et al., 2014) website.

Here are some predicted properties of the molecules above:

Molecule 1

SMILES Formula: CN[C@@H]1CC2(COC2)CC3[C@@H]1Nc4cccc5c4N3CC(C5)F Molecular Formula: $C_{18}H_{24}FN_{3}O$ Formula Weight: 317.4010632 Composition: C(68.11%) H(7.62%) F(5.99%) N(13.24%) O(5.04%) Molar Refractivity: 87.10 ± 0.4 cm³ Molar Volume: 246.3 ± 5.0 cm³ Parachor: 663.3 ± 6.0 cm³ Index of Refraction: 1.624 ± 0.03 Surface Tension: 52.5 ± 5.0 dyne/cm Density: 1.28 ± 0.1 g/cm³ Polarizability: 34.52 ± 0.5 10⁻²⁴cm³ RDBE: 8 Monoisotopic Mass: 317.190341 Da Nominal Mass: 317 Da Average Mass: 317.4011 Da M+: 317.189792 Da M-: 317.190889 Da [M+H]+: 318.197617 Da [M+H]-: 318.198714 Da [M-H]+: 316.181967 Da [M-H]-: 316.183064 Da.

Molecule 2

SMILES Formula: C[C@@H](C(F)(F)F)Nc1cccc2c1NCC(C2)F Molecular Formula: C₁₂H₁₄F₄N₂ Formula Weight: 262.2465728 Composition: C(54.96%) H(5.38%) F(28.98%) N(10.68%) Molar Refractivity: 60.21 ± 0.4 cm³ Molar Volume: $206.6 \pm 5.0 \text{ cm}^3$ Parachor: 496.2 ± 6.0 cm³ Index of Refraction: 1.494 ± 0.03 Surface Tension: 33.2 ± 5.0 dyne/cm Density: $1.26 \pm 0.1 \text{ g/cm}^3$ Polarizability: 23.87 ± 0.5 10⁻²⁴ cm³ RDBE: 5 Monoisotopic Mass: 262.109311 Da Nominal Mass: 262 Da Average Mass: 262.2466 Da M+: 262.108763 Da M-: 262.10986 Da [M+H]+: 263.116588 Da [M+H]-: 263.117685 Da [M-H]+: 261.100938 Da [M-H]-: 261.102035 Da.

Molecule 3

SMILES Formula: FC(C1)CNc2c1cccc2N[C@@H]3C(O)CCCC3 Molecular Formula: C₁₅H₂₁FN₂O Formula Weight: 264.3384432 Composition: C(68.16%) H(8.01%) F(7.19%) N(10.60%) O(6.05%) Molar Refractivity: 73.21 ± 0.4 cm³ Molar Volume: 219.1 ± 5.0 cm³ Parachor: 578.2 ± 6.0 cm³ Index of Refraction: 1.582 ± 0.03 Surface Tension: 48.4 ± 5.0 dyne/cm Density: $1.20 \pm 0.1 \text{ g/cm}^3$ Polarizability: 29.02 ± 0.5 10⁻²⁴ cm³ RDBE: 6 Monoisotopic Mass: 264.163792 Da Nominal Mass: 264 Da Average Mass: 264.3384 Da M+: 264.163243 Da M-: 264.16434 Da [M+H]+: 265.171068 Da [M+H]-: 265.172165 Da [M-H]+: 263.155418 Da [M-H]-: 263.156515 Da.

Molecule 4

SMILES Formula: FC(C1)CNc2c1cccc2NCCCC Molecular Formula: C₁₃H₁₉FN₂ Formula Weight: 222.3017632 Composition: C(70.24%) H(8.61%) F(8.55%) N(12.60%) Molar Refractivity: 64.50 ± 0.4 cm³ Molar Volume: $206.6 \pm 5.0 \text{ cm}^3$ Parachor: $514.6 \pm 6.0 \text{ cm}^{3}$ Index of Refraction: 1.536 ± 0.03 Surface Tension: 38.4 ± 5.0 dyne/cm Density: $1.07 \pm 0.1 \text{ g/cm}^3$ Polarizability: 25.57 ± 0.5 10⁻²⁴ cm³ RDBE: 5 Monoisotopic Mass: 222.153227 Da Nominal Mass: 222 Da Average Mass: 222.3018 Da M+: 222.152678 Da M-: 222.153775 Da [M+H]+: 223.160503 Da [M+H]-: 223.1616 Da [M-H]+: 221.144853 Da [M-H]-: 221.14595 Da.

2. Materials and Methods

Through the internet sites and others references (Daina et al., 2017), (Daina et al., 2014), (Daina and Zoete, 2016) and (Nickel et al., 2014), we will study the molecules represented in Figures 1, 2, 3 and 4 above, in order to conclude that it is very promising in the fight against some diseases.

2.1. ADME parameters and others

As seen in Figure 5 and 7, the molecules are lead-likeness, passing through the criteria listed below, as well as having a bioavaliability score of 0.55. As seen in Figures 6 and 8, the molecules are drug-likeness, passing through the criteria listed below, as well as having a bioavaliability score of 0.55. For other information, just look at Annex 1, at the end of this paper.

2.2. The indications of predicted targets

The indication of predicted target for brain cancer is of 94.33% of probability and the model accuracy is of 82.69% of probability, see Fig. 9. The indication of predicted target for multiple sclerosis is of 95.13% of probability and the model accuracy is of 98.95% of probability, see Fig. 10. The indication of predicted target for ocular cancer is of 96.22% of probability and the model accuracy is of 98.71% of probability and the model accuracy is of 98.95% of probability and the model accuracy is of 98.71% of probability and the model accuracy is of 98.95% of probability, see Fig. 12. All in Annex 2, at the end of this paper.

3. Results and Discussion

The four molecules are very promising for the fight against some diseases, according to an *in silico* analysis carried out by the SuperPRED website (Nickel et al., 2014), with more than 90% chance of success in the compatibility between the target and the ligand. Besides, the molecules are free of toxicity, as attested by the *in silico* prediction in Annex 1, Figures 5, 6, 7 and 8, all below.

4. Conclusions

In the future, it is possible to do molecular docking, as well as discover new molecules analogous to the one given above.

5. References

- Daina, A., Michielin, O., Zoete, V., 2017. SwissADME: a free web tool to evaluate pharmacokinetics, druglikeness and medicinal chemistry friendliness of small molecules. Sci. Rep. 7, 1–13. https://doi.org/10.1038/srep42717.
- Daina, A., Michielin, O., Zoete, V., 2014. iLOGP: A Simple, Robust, and Efficient Description of n-Octanol/Water Partition Coefficient for Drug Design Using the GB/SA Approach | Journal of Chemical Information and Modeling. J. Chem. Inf. Model. 54, 3284–3301. https://doi.org/10.1021/ci500467k.
- Daina, A., Zoete, V., 2016. A BOILED-Egg To Predict Gastrointestinal Absorption and Brain Penetration of Small Molecules. ChemMedChem 11, 1117–1121. https://doi.org/10.1002/cmdc.201600182.
- Nickel, J., Gohlke, B.-O., Erehman, J., Banerjee, P., Rong, W.W., Goede, A., Dunkel, M., Preissner, R., 2014. SuperPred: update on drug classification and target prediction. Nucleic Acids Res. 42, W26–W31. https://doi.org/10.1093/nar/gku477.

6. Annexs

Annex 1

Molecule 1			
#⊙⊙₽			Water Solubility
	LIPO	Log S (ESOL) 🤨	-3.35
H ² C NH		Solubility	1.41e-01 mg/ml ; 4.44e-04 mol/l
н	FLEX SIZE	Class 0	Soluble
NIII.		Log S (Ali) 🧐	-2.65
FT LA		Solubility	7.05e-01 mg/ml ; 2.22e-03 mol/l
		Class 0	Soluble
TI			
\checkmark	INSATU POLAR	Log S (SILICOS-IT)	-4.33
		Solubility	1.48e-02 mg/ml ; 4.86e-05 mol/l
F	INSOLU	Class 🥹	Moderately soluble
	1100.0		Pharmacokinetics
SMILES CN[C@@H]1CC2	2(COC2)CC2[C@@H]1Nc1cccc3c1N2CC(C3)F	GI absorption 🤨	High
Ph	ysicochemical Properties	BBB permeant 🧐	Yes
Formula	C18H24FN3O	P-gp substrate 🧐	Yes
Molecular weight	317.40 g/mol	CYP1A2 inhibitor 🤨	No
Num. heavy atoms	23	CYP2C19 inhibitor	No
Num. arom. heavy atoms	6	CYP2C9 inhibitor 🤨	No
Fraction Csp3	0.67	CYP2D6 inhibitor 🎯	Yes
Num. rotatable bonds	1	CYP3A4 inhibitor 😣	No
Num. H-bond acceptors	3	Log K_p (skin permeation) 60	-6.64 cm/s
Num. H-bond donors	2	r.	Druglikeness
Molar Refractivity	94.47	Lipinski 😣	Yes; 0 violation
TPSA 🤨	36.53 Ų	Ghose	Yes
	Lipophilicity	Veber 😣	Yes
Log P _{a/w} (iLOGP) 🌕	2.58	Egan 🛞	Yes
Log P _{a/w} (XLOGP3) 😣	2.25	Muegge 📀	Yes
Log P _{a/w} (WLOGP) 🤨	1.42	Bioavailability Score 📀	0.55
Log Poly (MLOGP)	2.19		Medicinal Chemistry
Log P _{o/w} (SILICOS-IT) 8	1.86	PAINS 😣	0 alert
Consensus Log Poly 0	2.06	Brenk 🛞	0 alert
Consensus Log Fo/W	2.00	Leadlikeness 😣	Yes
		Synthetic accessibility 🌕	4.51

Fig. 5. ADME parameters and others of the molecule $C_{18}H_{24}FN_3O$. Source: *http://www.swissadme.ch.*

Molecule 2				
Ħ⊕⊜ <i>₽</i>			Water Solubility	
	LIPO	Log S (ESOL) 🤨	-3.96	
i i		Solubility	2.88e-02 mg/ml ; 1.10e-04 mol/l	
FF	FLEX	Class 😣	Soluble	
\rightarrow		Log S (Ali) 🧐	-4.08	
н₂стрин		Solubility	2.17e-02 mg/ml ; 8.27e-05 mol/l	
		Class 😣	Moderately soluble	
	INSATU POLAR	Log S (SILICOS-IT) 🤨	-4.70	
		Solubility	5.18e-03 mg/ml ; 1.98e-05 mol/l	
\sim \sim	F	Class 😣	Moderately soluble	
	INSOLU		Pharmacokinetics	
SMILES FC1CNc2c(C1)cc	cc2N[C@H](C(F)(F)F)C	GI absorption 🤨	High	
	ysicochemical Properties	BBB permeant 🧐	Yes	
Formula	C12H14F4N2	P-gp substrate 🧐	No	
Molecular weight	262.25 g/mol	CYP1A2 inhibitor Օ	No	
Num. heavy atoms	18	CYP2C19 inhibitor 😣	No	
Num. arom. heavy atoms	6	CYP2C9 inhibitor 🤨	No	
Fraction Csp3	0.50	CYP2D8 inhibitor 🧐	Yes	
Num. rotatable bonds	3	CYP3A4 inhibitor 😣	No	
Num. H-bond acceptors	4	Log K_p (skin permeation) $^{(0)}$	-5.14 cm/s	
Num. H-bond donors	2	Druglikeness		
Molar Refractivity	65.50	Lipinski 🔞	Yes; 0 violation	
TPSA 😣	24.08 Ų	Ghose 🛞	Yes	
	Lipophilicity	Veber 😣	Yes	
Log P _{a/w} (iLOGP) 🌕	2.00	Egan 🕖	Yes	
Log P _{o/w} (XLOGP3) 🥹	3.88	Muegge 📀	Yes	
Log P _{o/w} (WLOGP) 🤨	4.27	Bioavailability Score 🥺	0.55	
Log P _{o/w} (MLOGP) 😣	2.82		Medicinal Chemistry	
Log Poly (SILICOS-IT)	3.12	PAINS	0 alert	
Consensus Log Pow ⁽⁰⁾	3.22	Brenk 🛞	0 alert	
Consensus Log P _{O/W}	3.22	Leadlikeness Θ	No; 1 violation: XLOGP3>3.5	
		Synthetic accessibility 🌕	2.87	

Fig. 6. ADME parameters and others of the molecule $C_{12}H_{14}F_4N_2$. Source: http://www.swissadme.ch.

Molecule 3			
₩ ⊕ () <i>@</i>			Water Solubility
	LIPO	Log S (ESOL) 🤨	-3.48
		Solubility	9.08e-02 mg/ml ; 3.43e-04 mol/l
T TI	FLEX SIZE	Class 😣	Soluble
		Log S (Ali) 🤨	-3.58
N T		Solubility	6.89e-02 mg/ml ; 2.61e-04 mol/l
N	4	Class 😣	Soluble
		Log S (SILICOS-IT) 19	-4.01
	INSATU POLAR	Solubility	2.57e-02 mg/ml ; 9.71e-05 mol/l
	4	Class 0	Moderately soluble
	INSOLU		Pharmacokinetics
		GI absorption 0	High
SMILES FC1CNc2c(C1)cc		BBB permeant 0	Yes
Formula	vsicochemical Properties C15H21FN2O	P-gp substrate ⁽⁹⁾	Yes
Molecular weight	264.34 g/mol	CYP1A2 inhibitor 0	No
Num. heavy atoms	19	CYP2C19 inhibitor 8	No
Num. arom. heavy atoms	6	CYP2C9 inhibitor 9	No
Fraction Csp3	0.60	CYP2D6 inhibitor 0	Yes
Num. rotatable bonds	2	CYP3A4 inhibitor 0	Ne
Num. H-bond acceptors	2	Log K_n (skin permeation) 0	-5.79 cm/s
Num. H-bond donors	3	Druglikeness	
Molar Refractivity	78.78	Lipinski 😣	Yes: 0 violation
TPSA 0	44.29 Ų	Ghose 😣	Yes
	Lipophilicity	Veber 😣	Yes
Log P _{o/w} (iLOGP) 🤨	2.41	Egan 0	Yes
Log P _{olw} (XLOGP3) 🥹	2.99	Muegge 🥹	Yes
Log Poly (WLOGP)	2.37	Bioavailability Score 0	0.55
Log Poly (MLOGP)	2.32		Medicinal Chemistry
Log Poly (SILICOS-IT)	2.34	PAINS 😣	0 alert
Consensus Log P _{o/w} ⁽⁰⁾		Brenk 😣	0 alert
Consensus Log P _{0/W}	2.49	Leadlikeness 🔞	Yes
		Synthetic accessibility 🧐	3.37

Fig. 7. ADME parameters and others of the molecule $C_{15}H_{21}FN_2O$. Source: *http://www.swissadme.ch.*

Molecule 4				
₩ ⊕ ○ <i>@</i>			Water Solubility	
	LIPO	Log S (ESOL) 🤨	-3.49	
		Solubility	7.14e-02 mg/ml ; 3.21e-04 mol/l	
	CH, FLEX SIZE	Class ()	Soluble	
ÍÌ		Log S (Ali) 🤨	-3.78	
		Solubility	3.67e-02 mg/ml ; 1.65e-04 mol/l	
	K	Class 🛞	Soluble	
\searrow	INSATU	Log S (SILICOS-IT) 😣	-4.99	
	Poon Poon	Solubility	2.29e-03 mg/ml ; 1.03e-05 mol/l	
		Class 0	Moderately soluble	
	INSOLU		Pharmacokinetics	
SMILES CCCCNc1cccc2c	1NCC(C2)E	GI absorption 📀	High	
	ysicochemical Properties	BBB permeant 😣	Yes	
Formula	C13H19FN2	P-gp substrate 🧐	No	
Molecular weight	222.30 g/mol	CYP1A2 inhibitor 🔞	Yes	
Num. heavy atoms	16	CYP2C19 inhibitor 😣	No	
Num. arom. heavy atoms	6	CYP2C9 inhibitor 🧐	No	
Fraction Csp3	0.54	CYP2D6 inhibitor 📀	Yes	
Num. rotatable bonds	4	CYP3A4 inhibitor 😣	No	
Num. H-bond acceptors	1	Log K _n (skin permeation) 📀	-5.11 cm/s	
Num. H-bond donors	2	Druglikeness		
Molar Refractivity	70.12	Lipinski 😗	Yes: 0 violation	
TPSA 🛞	24.06 Ų	Ghose 8	Yes	
	Lipophilicity	Veber	Yes	
Log P _{a/w} (iLOGP) 🤨	2.69	Egan 🔞	Yes	
Log P _{o/w} (XLOGP3) 😣	3.59	Muegge 🥹	Yes	
Log P _{o/w} (WLOGP) 😣	2.86	Bioavailability Score 0	0.55	
Log Poly (MLOGP)	2.68	-	Medicinal Chemistry	
Log Poly (SILICOS-IT)	3.10	PAINS	0 alert	
		Brenk 😣	0 alert	
Consensus Log P _{o/w} 😣	2.99	Leadlikeness 🛞	No; 2 violations: MW<250, XLOGP3>3.5	
		Synthetic accessibility 🌕	2.72	

Fig. 8. ADME parameters and others of the molecule $C_{13}H_{19}FN_2$. Source: http://www.swissadme.ch.

Annex	2
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Target Name 🔶	ChEMBL- ID	Indication \diamond	Probability •	Model 🔶 accuracy
Signal transducer and activator of transcription 3	T29130	Brain cancer [ICD-11: 2A00]	94.33%	82.69%
Signal transducer and activator of transcription 3	T29130	Chronic lymphocytic leukaemia [ICD-11: 2A82.0]	94.33%	82.69%
Signal transducer and activator of transcription 3	T29130	Hepatocellular carcinoma [ICD-11: 2C12.02]	94.33%	82.69%
Signal transducer and activator of transcription 3	T29130	Immune System disease [ICD-11: 4A01- 4B41]	94.33%	82.69%
Signal transducer and activator of transcription 3	T29130	Inflammation [ICD-11: 1A00-CA43.1]	94.33%	82.69%
Signal transducer and activator of transcription 3	T29130	Multiple myeloma [ICD-11: 2A83]	94.33%	82.69%
Signal transducer and activator of transcription 3	T29130	Psoriasis vulgaris [ICD-11: EA90]	94.33%	82.69%
Signal transducer and activator of transcription 3	T29130	Recurrent glioblastoma [ICD-11: 2A00.00]	94.33%	82.69%
Signal transducer and activator of transcription 3	T29130	Solid tumour/cancer [ICD-11: 2A00-2F9Z]	94.33%	82.69%
Signal transducer and activator of transcription 3	T29130	Ulcerative colitis [ICD-11: DD71]	94.33%	82.69%

Fig. 9. Indications of predicted target of the molecule $C_{18}H_{24}FN_3O$. Source: https://prediction.charite.de/subpages/target_prediction.php

Target Name	ChEMBL-	Indication \diamond	Probability 🔹	Model
Cathepsin D	T67102	Hypertension [ICD-11: BA00-BA04]	95.13%	98.95%
Cathepsin D	T67102	Multiple sclerosis [ICD-11: 8A40]	95.13%	98.95%
Neuronal acetylcholine receptor; alpha3/beta4	T73724	Alzheimer disease [ICD-11: 8A20]	94.82%	97.23%
Neuronal acetylcholine receptor; alpha3/beta4	T73724	Tobacco dependence [ICD-11: 6C4A.2]	94.82%	97.23%
DNA-(apurinic or apyrimidinic site) Iyase	T13348	Glioma [ICD-11: 2A00.0]	92.4%	91.11%
DNA-(apurinic or apyrimidinic site) lyase	T13348	Melanoma [ICD-11: 2C30]	92.4%	91.11%
DNA-(apurinic or apyrimidinic site) Iyase	T13348	Ocular cancer [ICD-11: 2D00-2D07]	92.4%	91.11%
DNA-(apurinic or apyrimidinic site) Iyase	T13348	Solid tumour/cancer [ICD-11: 2A00- 2F9Z]	92.4%	91.11%
G-protein coupled receptor 55	T87670	Attention deficit hyperactivity disorder [ICD-11: 6A05.Z]	90.62%	78.15%
PI3-kinase p110-beta subunit	T05031	Breast cancer [ICD-11: 2C60-2C65]	90.06%	98.75%

Fig. 10. Indications of predicted target of the molecule $C_{12}H_{14}F_4N_2$. Source: *https://prediction.charite.de/subpages/target_prediction.php*

Target Name	ChEMBL- ID	Indication \diamond	Probability -	Model accuracy
DNA-(apurinic or apyrimidinic site) lyase	T13348	Glioma [ICD-11: 2A00.0]	96.22%	91.11%
DNA-(apurinic or apyrimidinic site) lyase	T13348	Melanoma [ICD-11: 2C30]	96.22%	91.11%
DNA-(apurinic or apyrimidinic site) lyase	T13348	Ocular cancer [ICD-11: 2D00-2D07]	96.22%	91.11%
DNA-(apurinic or apyrimidinic site) lyase	T13348	Solid tumour/cancer [ICD-11: 2A00-2F9Z]	96.22%	91.11%
Adenosine A1 receptor	T92072	Acute and chronic heart failure [ICD-11: BD1Z]	96.11%	95.93%
Adenosine A1 receptor	T92072	Allergy [ICD-11: 4A80-4A85]	96.11%	95.93%
Adenosine A1 receptor	T92072	Atrial fibrillation [ICD-11: BC81.3]	96.11%	95.93%
Adenosine A1 receptor	T92072	Autoimmune diabetes [ICD-11: 5A10]	96.11%	95.93%
Adenosine A1 receptor	T92072	Cardiac arrhythmias [ICD-11: BC9Z]	96.11%	95.93%
Adenosine A1 receptor	T92072	Cardiac disease [ICD-11: BA00-BE2Z]	96.11%	95.93%

Fig. 11. Indications of predicted target of the molecule $C_{15}H_{21}FN_2O$. Source: *https://prediction.charite.de/subpages/target_prediction.php*

Target Name	¢	ChEMBL- ID	Indication ÷	Probability 🗸	Model accuracy
Cathepsin D		T67102	Hypertension [ICD-11: BA00-BA04]	98.71%	98.95%
Cathepsin D		T67102	Multiple sclerosis [ICD-11: 8A40]	98.71%	98.95%
HERG		T20251	Angina pectoris [ICD-11: BA40]	93.42%	89.76%
HERG		T20251	Cardiac arrhythmias [ICD-11: BC9Z]	93.42%	89.76%
HERG		T20251	Cardiac failure [ICD-11: BD10-BD13]	93.42%	89.76%
HERG		T20251	Heart arrhythmia [ICD-11: BC65]	93.42%	89.76%
HERG		T20251	Malaria [ICD-11: 1F40-1F45]	93.42%	89.76%
HERG		T20251	Multiple sclerosis [ICD-11: 8A40]	93.42%	89.76%
HERG		T20251	Ovarian cancer [ICD-11: 2C73]	93.42%	89.76%
HERG		T20251	Pain [ICD-11: MG30-MG3Z]	93.42%	89.76%

Fig. 12. Indications of predicted target of the molecule $C_{13}H_{19}FN_2.$ Source: <code>https://prediction.charite.de/subpages/target_prediction.php</code>