Figure 1: LogP histogram of benzylidene-acrylohydrazide derivatives (n=69) synthesized by Giancotti and colleagues [30].

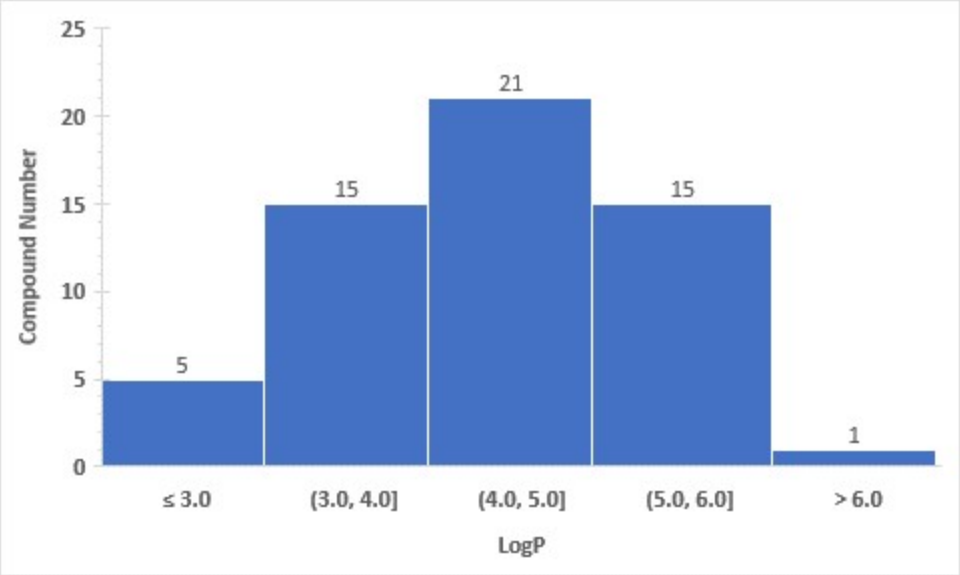


Figure 2: Permeability in the blood-brain barrier (BBB) histogram of benzylidene-acrylohydrazide derivatives (n=69) synthesized by Giancotti and colleagues [30].

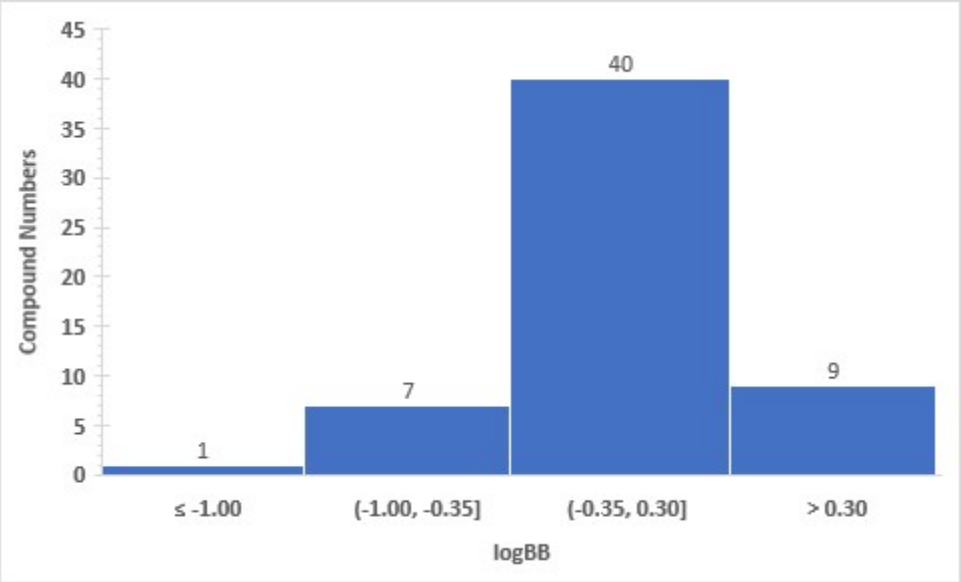


Figure 3: Brain permeability (logPS) histogram of benzylidene-acrylohydrazide derivatives (n=69) synthesized by Giancotti and colleagues [30].

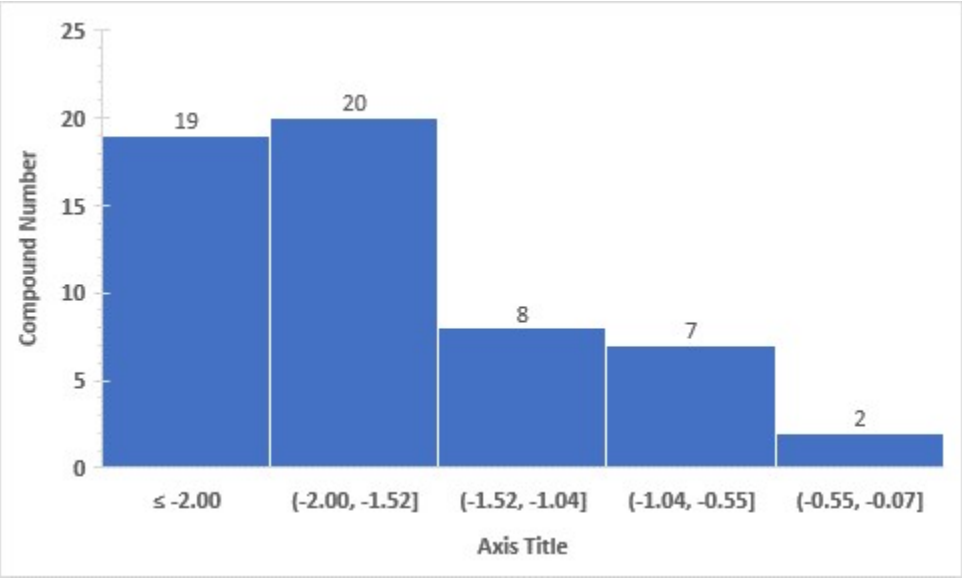
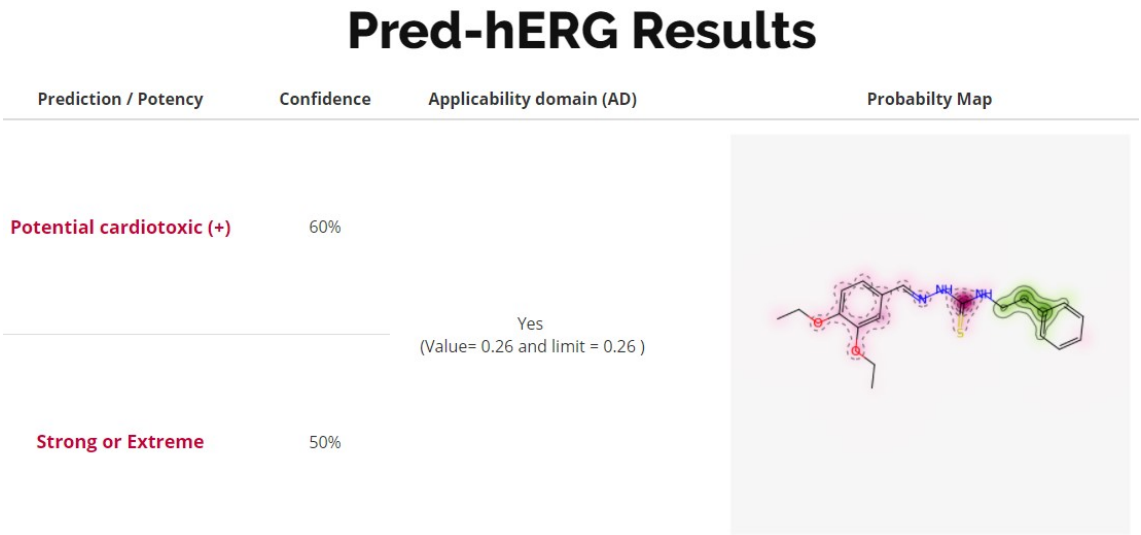


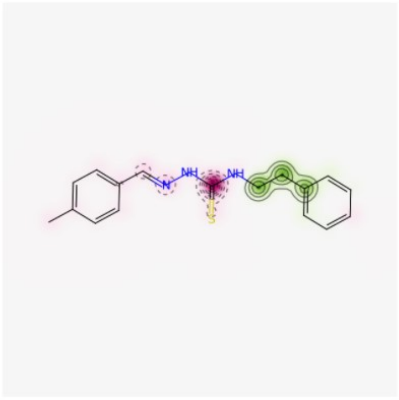
Figure 4: Cardiotoxicity prediction of benzylidene-acrylohydrazide derivatives synthesized by Giancotti and colleagues [30] that presented higher values (strong) determined by PREDHERG 4.2 [32] (http://predherg.labmol.com.br/). A) 41, B) 42, C) 43, D) 44, E) 77, F) 78, G) 79, H) 80 and I) 93.

A)



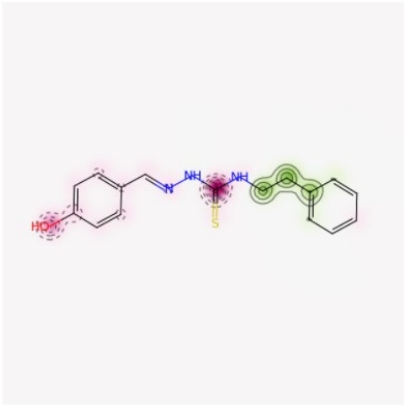
B)

Pred-hERG Results

Prediction / Potency	Confidence	Applicability domain (AD)	Probabilty Map
Potential cardiotoxic (+)	60%	Yes (Value= 0.26 and limit = 0.26)	
Strong or Extreme	60%		

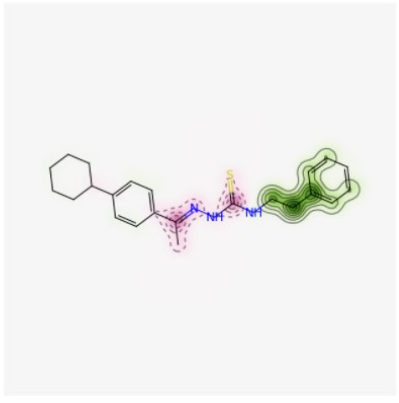
C)

Pred-hERG Results

Prediction / Potency	Confidence	Applicability domain (AD)	Probabilty Map
Potential cardiotoxic (+)	60%	Yes (Value= 0.26 and limit = 0.26)	
Strong or Extreme	60%		

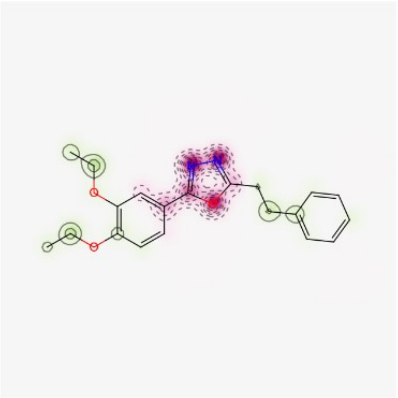
D)

Pred-hERG Results

Prediction / Potency	Confidence	Applicability domain (AD)	Probabilty Map
Potential cardiotoxic (+)	60%	Yes (Value= 0.27 and limit = 0.26)	
Strong or Extreme	60%		

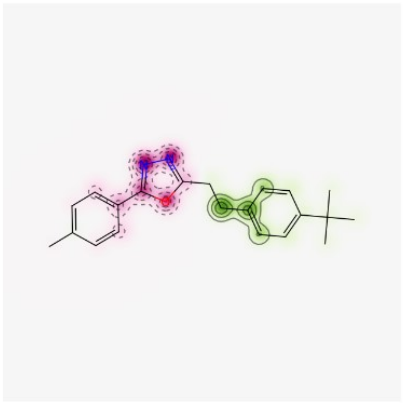
E)

Pred-hERG Results

Prediction / Potency	Confidence	Applicability domain (AD)	Probabilty Map
Potential cardiotoxic (+)	60%	Yes (Value= 0.27 and limit = 0.26)	
Strong or Extreme	50%		

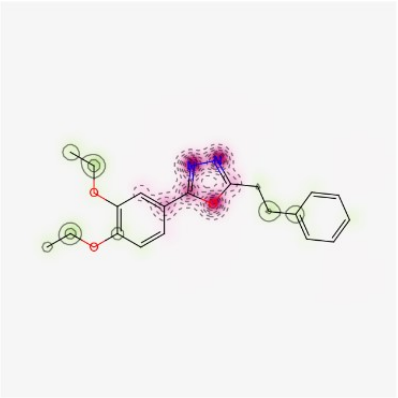
F)

Pred-hERG Results

Prediction / Potency	Confidence	Applicability domain (AD)	Probabilty Map
Potential cardiotoxic (+)	60%	No (Value= 0.25 and limit = 0.26)	
Strong or Extreme	50%		

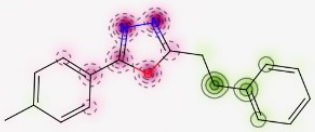
G)

Pred-hERG Results

Prediction / Potency	Confidence	Applicability domain (AD)	Probabilty Map
Potential cardiotoxic (+)	60%	Yes (Value= 0.27 and limit = 0.26)	
Strong or Extreme	50%		

H)

Pred-hERG Results

Prediction / Potency	Confidence	Applicability domain (AD)	Probabilty Map
Potential cardiotoxic (+)	60%	Yes (Value= 0.27 and limit = 0.26)	
Strong or Extreme	60%		

I)

Pred-hERG Results

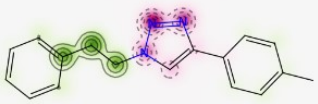
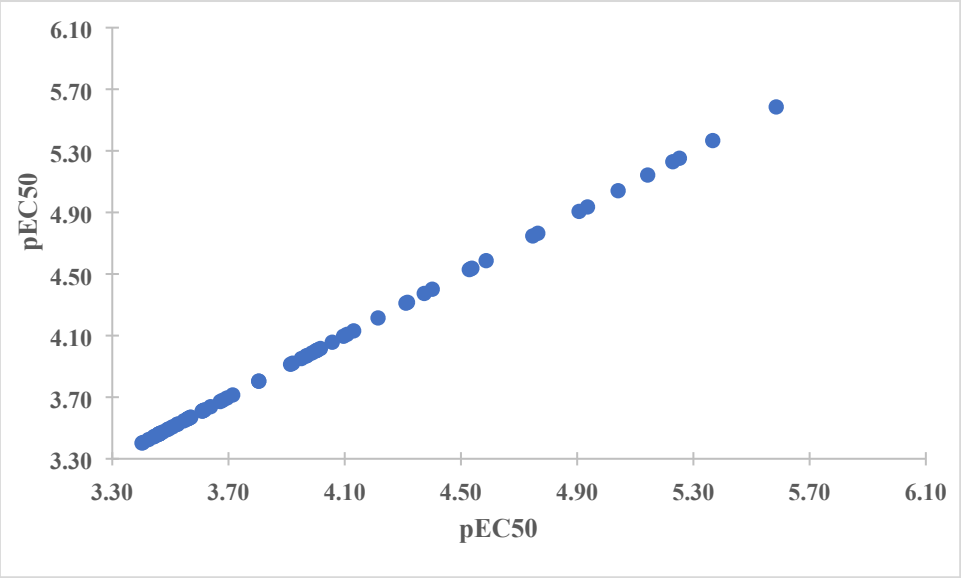
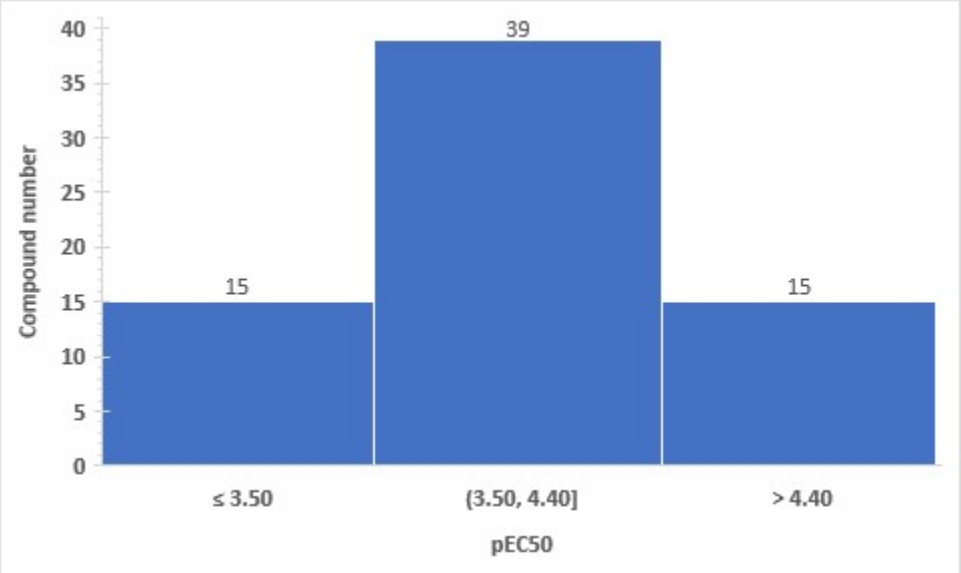
Prediction / Potency	Confidence	Applicability domain (AD)	Probabilty Map
Potential cardiotoxic (+)	70%	Yes (Value= 0.3 and limit = 0.26)	
Strong or Extreme	60%		

Figure 5: Biological activities (pEC50) data of benzylidene-acrylohydrazide derivatives (n=69) synthesized by Giancotti and colleagues [30]. A) pEC50 distribution and B) pEC50 histogram

A)


6.10
5.70
5.30
4.90
4.50
4.10
3.70
3.30
pEC50
3.30
3.70
4.10
4.50
4.90
5.30
5.70
6.10
pEC50

B)


40
35
30
25
20
15
10
5
0
Compound number
15
39
15
≤ 3.50
(3.50, 4.40]
> 4.40
pEC50