



FACULTY OF PHARMACY  
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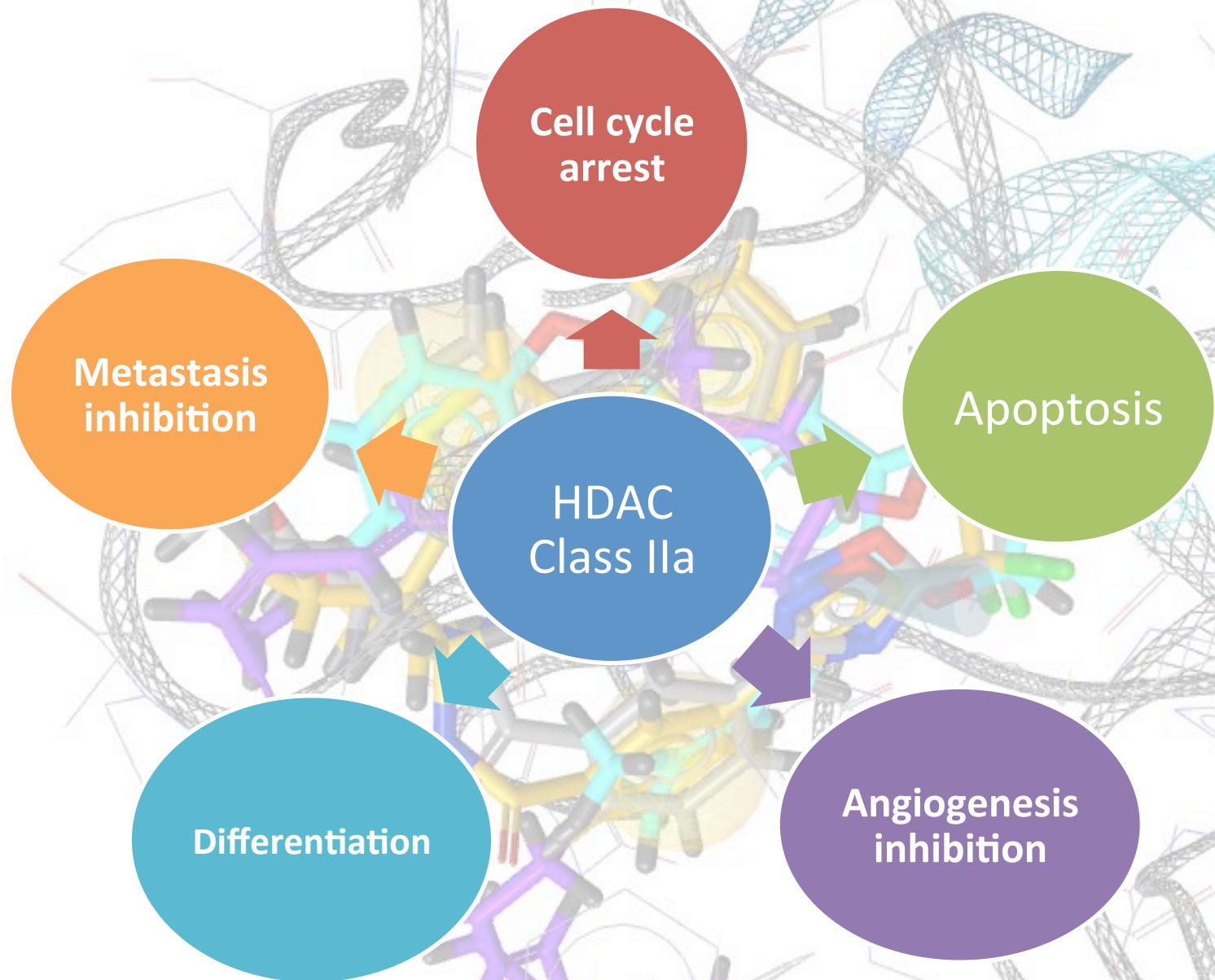
# VIRTUAL SCREENING OF INDONESIAN HERBAL DATABASE AS AN ACTIVE LIGAND FOR HDAC4 AND HDAC7 BASED ON PHARMACOPHORE APPROACHED

Linda Erlina, Azminah, Andika, and Arry Yanuar\*

Email Corresponding Author (\*):  
[arry.yanuar@ui.ac.id](mailto:arry.yanuar@ui.ac.id)

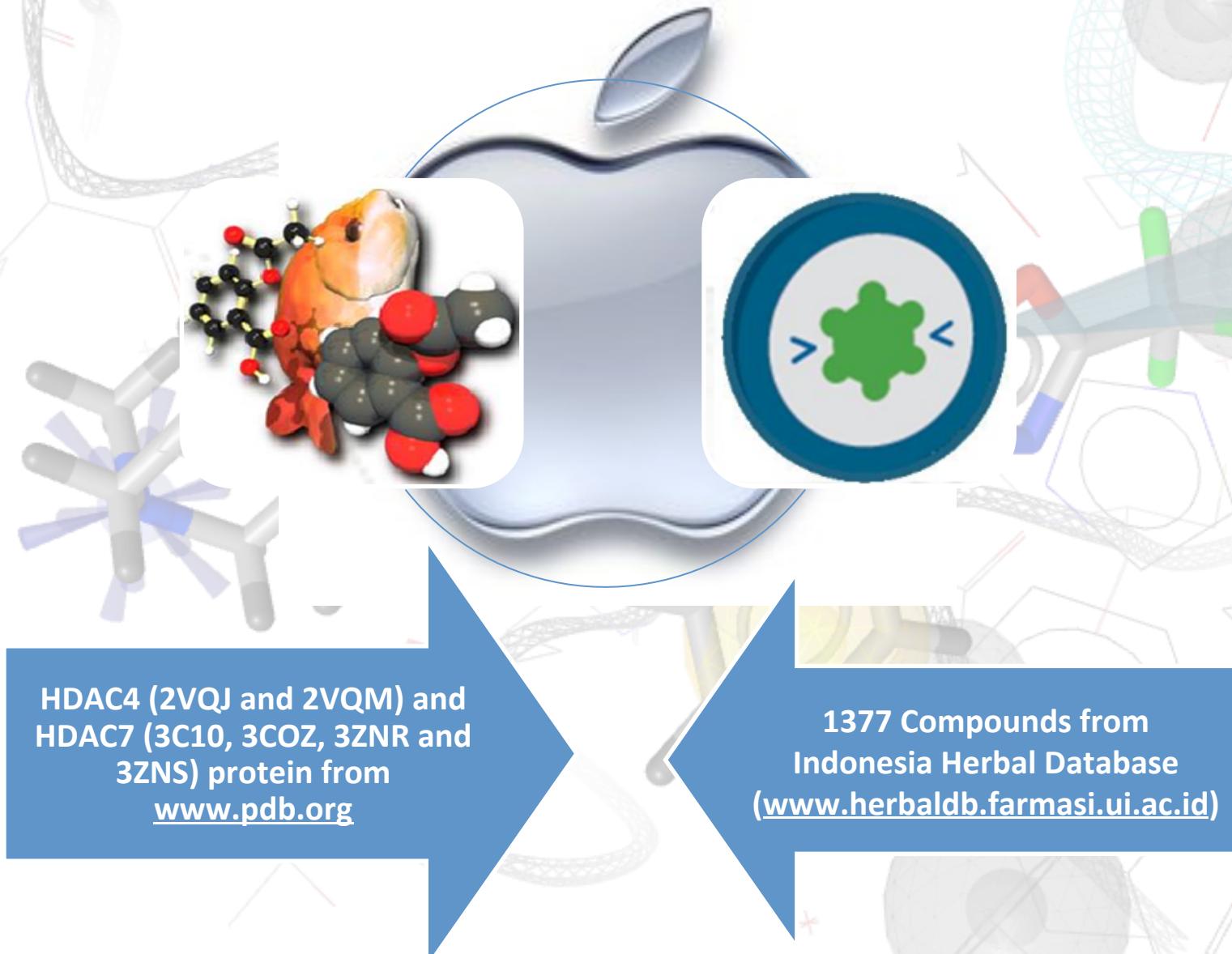


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Depok—Indonesia



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# Instruments and Materials

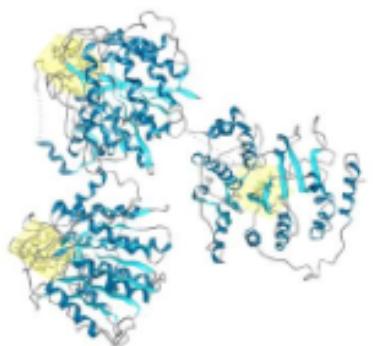


HDAC4 (2VQJ and 2VQM) and HDAC7 (3C10, 3COZ, 3ZNR and 3ZNS) protein from [www.pdb.org](http://www.pdb.org)

1377 Compounds from Indonesia Herbal Database ([www.herbaldb.farmasi.ui.ac.id](http://www.herbaldb.farmasi.ui.ac.id))

## Work Scheme

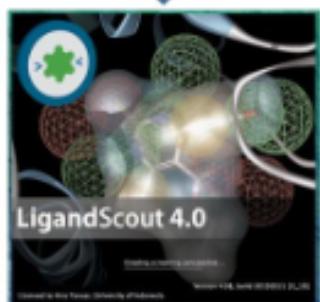
HDAC4 and HDAC7 Protein  
from [www.pdb.org](http://www.pdb.org)



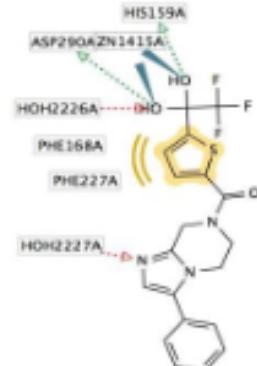
Compounds (.mol2) from  
[herbaldb.farmasi.ui.ac.id](http://herbaldb.farmasi.ui.ac.id)



Virtual Screening  
Omitted 0

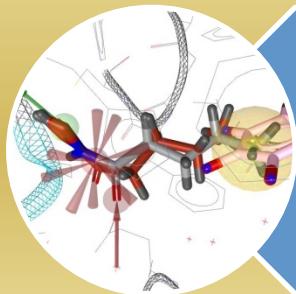


Re-docking using  
AutoDock Vina

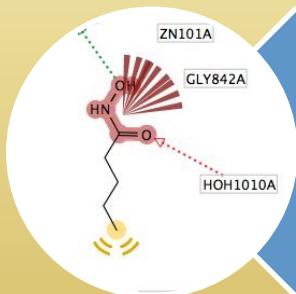


Hit Compounds

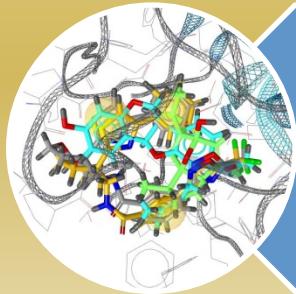
# Results and Discussion



Hit of Compounds



Core  
Pharmacophore



Re-docking

Name	PDB Code	Pharmacophore-Fit Score
Kaempferol 3-neohesperidoside	2VQJ	76,56
Mesuein	2VQJ	77,57
Glucoputranjivin	3COZ_A	45,74
Benzylglucosinolate	3COZ_A	
Sinigrin		
8-Methylthiophenoxy-		
3-Butenylglu-		
8-Hydroxyapigenin 8-(2'',4''-disulfatoglucuronide)	3COZ_A	46,14
Myricetin 3-(2G-rhamnosyl)-glucoside	3COZ_A	45,86
5-Hexenyl glucoside		
4-Methylpentyl glucoside		
3-Methylpentyl glucosinolate		
9-Methylthiononyl glucosinolate	3COZ_A	
1-Hexyl glucosinolate	3COZ_A	
Torvanol A	3COZ_A	45,86
Cent-Copalyl diphosphate	3COZ_C	46,78
Myristicanol A	3COZ_C	46,39
DIMBOA glucoside	3COZ_C	47,43
Myristicanol B	3COZ_C	46,39

Name	PDB Code	Pharmacophore-Fit Score
Geraniol	3ZNR	46,24
Cristacarpin	3ZNR	46,62
5-HETE	3ZNR	45,97
Guaiol	3ZNR	46,11
trans,trans-Farnesol	3ZNR	45,87
(Z,Z,Z)-3,6,9-Dodecatrien-1-ol	3ZNR	46,43
Nerolidol	3ZNR	46,58
Anacyclin	3ZNR	46,29

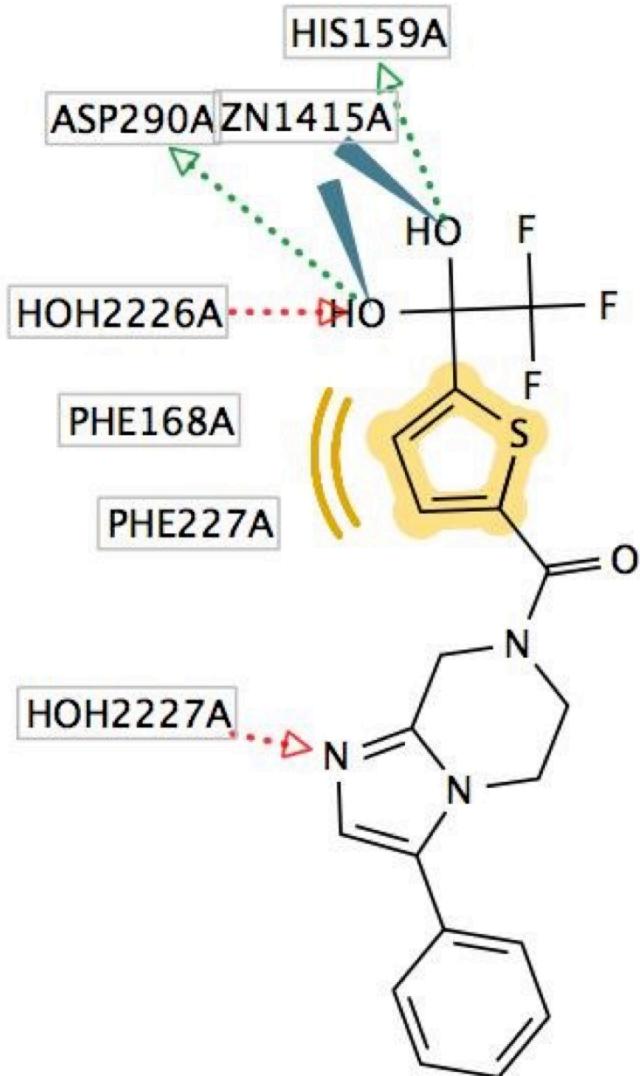
**Pellitorine**

**3ZNR**

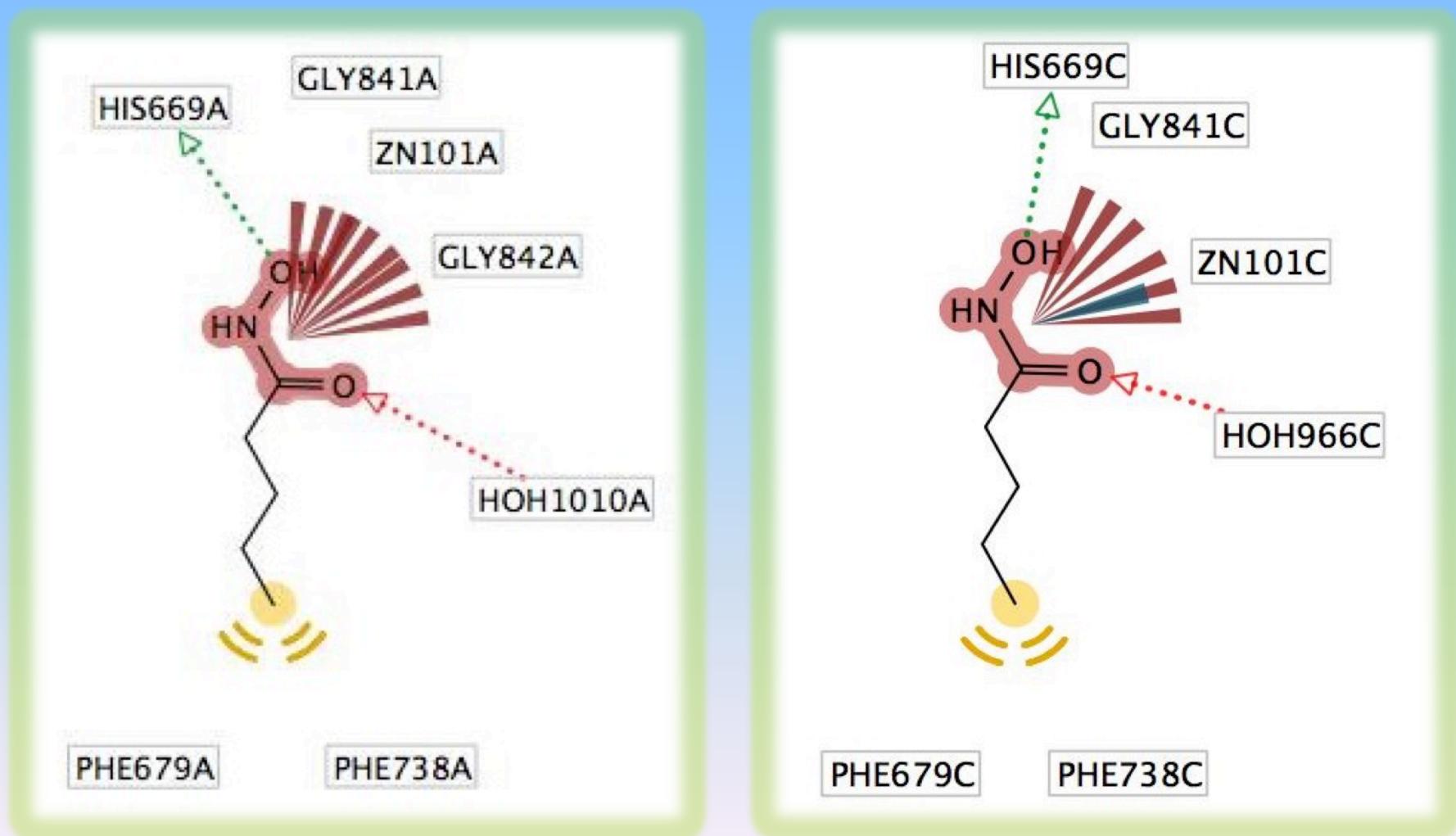
**46,73**

Violaxanthin	3ZNR	46,06
(Z)-2-Methyl-6-methylene-2,7-octadien-1-ol	3ZNR	46,00
Oxycurcumenol	3ZNR	46,51
Viridiflorol	3ZNR	45,42
Isovetiselinol	3ZNR	45,34
Pellitorine	3ZNR	46,73
(-)Oblongine	3ZNR	46,35
Guineensine	3ZNR	46,17
Marmin	3ZNR	46,22
Spilanthol	3ZNR	46,19

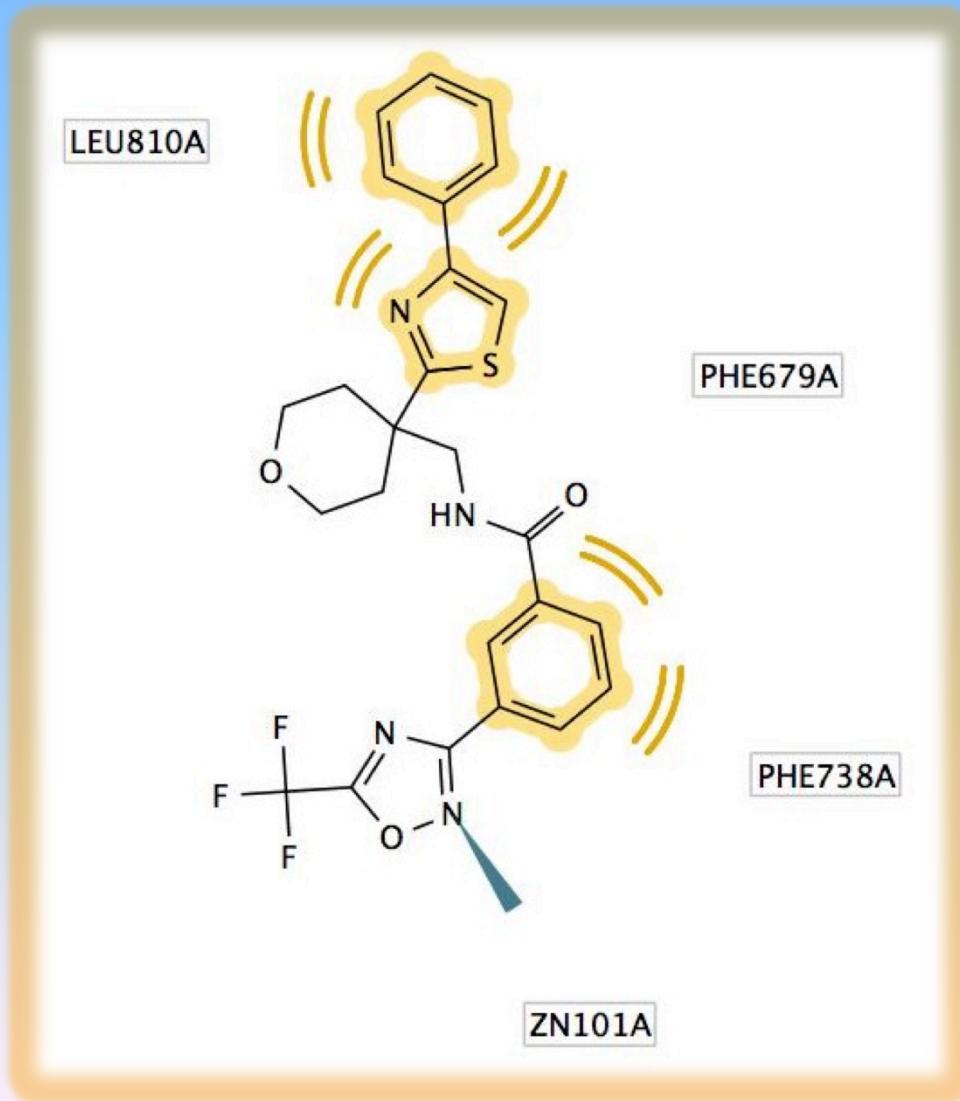
# Trimethyl Fluoro Ketone Pharmacophore (2VQJ)



# SAHA Pharmacophore (3COZ)

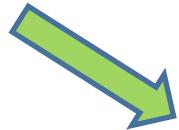


# TMP269 Pharmacophore (3ZNR)



# Re-docking hit compounds against 2VQJ

Name	Affinity (kcal/mol)
(2VQJ) [A] TFG1414	-9,3
Mesuein.mol	-9,8
Kaempferol 3-neohesperidoside.mol	-9,9



Name	Affinity (kcal/mol)
(3C0Z) [A] SHH301	-5,5
n-Hexyl glucosinolate.mol	-6,5
3-Methylpentyl glucosinolate.mol	-5,9
Glucoputranjivin.mol	-6,2
Sinigrin.mol	-7,3
8-Hydroxyapigenin 8-(2'',4''-disulfatoglucuronide).mol	-7,2
Torvanol A.mol	-7,2
3-Butenylglucosinolate.mol	-6,6
Benzylglucosinolate.mol	-6,7
8-Methylthio-octyl glucosinolate.mol	-5,9
5-Hexenyl glucosinolate.mol	-6,4
Myricetin 3-(2G-rhamnosylrutinoside).mol	-8,1

Re-docking hit  
compounds against  
3COZ\_A&B

Name	Affinity (kcal/mol)
(3C0Z) [C] SHH301	-5,4
DIMBOA glucoside.mol	-8,1
Benzylglucosinolate.mol	-7,8
Myristicanol B.mol	-7,3
Myristicanol A.mol	-6,9
ent-Copalyl diphosphate.mol	-7,9

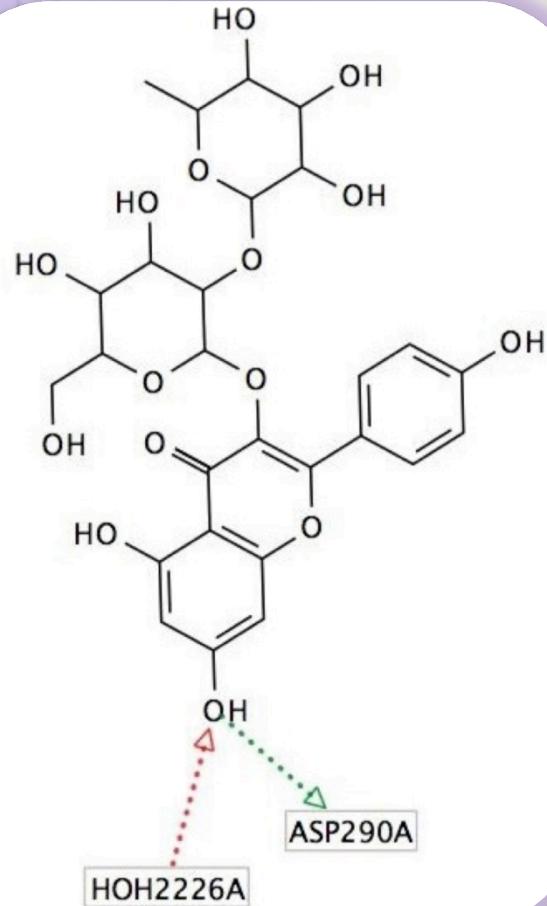
# Re-docking hit compounds against 3ZNR



Name	Affinity (kcal/mol)
Cristacarpin.mol	-10,1
nerolidol.mol	-7,3
Pellitorine.mol	-6,7
Oxycurcumenol.mol	-8
(Z,Z,Z)-3,6,9-Dodecatrien-1-ol.mol	-6,4
Phytol.mol	-6,4
(3ZNR) [A] NU91000	-11
Anacyclin.mol	-7,3
(-)-Oblongine.mol	-6,8
Geraniol.mol	-7,9
(Z)-2-Methyl-6-methylene-2,7-octadien-1-ol.mol	-6,3
Marmin.mol	-9,3
Spilanthol.mol	-6,8
trans,trans-Farnesol.mol	-7,4
5-HETE.mol	-7,1
Lutein.mol	-8,8

# Conclusions

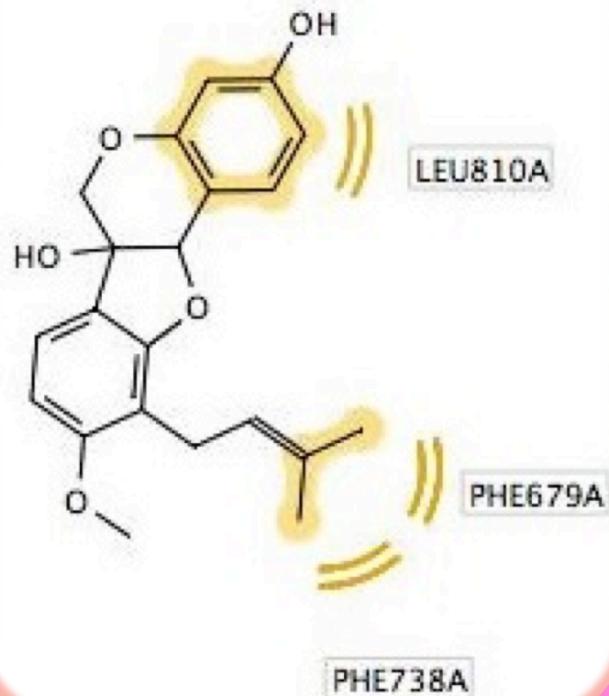
- The highest affinity as HDAC4 inhibitor is  
**Kampferol 3-neohespridoside**



# Conclusions

- The highest affinity as HDAC7 inhibitor is  
**Cristacarpin**

Cristacarpin.mol [1]



# References

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THANK  
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