Subject: How to calculate selectivity score?
Posted by jeetu270 on Fri, 30 Dec 2016 05:08:27 GMT
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Hi Thomas,

There is an option for calculating selectivity score in DataWarrior, which I think is Gini coefficient (if I am not wrong). I tried calculating this selectivity score for an inhibitor by giving the % residual kinase activities as the input column. But after running this calculation, its showing NaN in all the rows. Can you please guide me how to calculate this score since there is no help on this topic in your website.

Thanks for the great software..

Jitender

Subject: Re: How to calculate selectivity score?
Posted by thomas on Sat, 31 Dec 2016 16:24:55 GMT
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Hi Jitender,

I tried with some values and even empty cells, but always got numerical scores. There seems to be an issue, however, with logarithmical columns. The Gini logic should not be applied to logarithms, because the concept is 0-based. Currently, if a column is defined to be logarithmically treated, then then the Gini calculation uses the logarithms, which it shouldn't. I will solve that!

To solve your problem you may send me a data file and tell me which columns you use to generate the Gini score.

Regards, Thomas

Subject: Re: How to calculate selectivity score?
Posted by jeetu270 on Mon, 02 Jan 2017 04:02:11 GMT
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Thanks for the reply Thomas.

Actually as far as I understand the calculation of Gini score in the article, we need to input only a column containing the % residual activities for individual kinases. I tried with the example given in that paper (Table 1), and in their excel sheet only. It worked and calculated a single Gini score value. But the same % residual activities column (Column B) when I gave as input to DataWarrior, it showed Nan in all rows.

I am attaching the required files here, Please check..

Thanks
Jitender

Subject: Re: How to calculate selectivity score?
Posted by jeetu270 on Mon, 02 Jan 2017 04:31:20 GMT
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Hi Thomas,

Also I tried giving the % residual kinase activities for an inhibitor in a single row as shown in the attached excel file. It calculated and gave a Gini score value (0.25181) for the inhibitor but it is not matching with the one I calculated from the automated excel sheet provided by the author of the article (0.578)?

I think I am not providing the input in the right manner. Please help.

Thanks
Jitender

File Attachments
1) Gini_Coefficient_Calculation.dwar, downloaded 1097 times
2) Residual Activities_Transposed.xlsx, downloaded 959 times

Subject: Re: How to calculate selectivity score?
Posted by thomas on Sun, 05 Feb 2017 21:36:10 GMT
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Hi Jitender,

sorry for the late reply. I checked the paper, your files and the current Gini calculation method in DataWarrior. The main reason for the discrepancy is that the sample file from the paper contains effect values. Their published method converts them into inhibitions by basically inverting the values (inhibition=100-effect). Then they limit the value range by replacing any value beyond the allowed range (0-100) to the respective range limit (100 or 0). Into the bargain my method of calculating the areas was a little different. I changed my code to use their so-called trapez method. I also have a new option to invert the data (100-x). However, I will not do the correction to move values into the allowed range, because that would remove part of the noise in an unsymmetrical fashion. The update is due soon.

Thomas

Subject: Re: How to calculate selectivity score?

Posted by jeetu270 on Mon, 06 Feb 2017 08:21:01 GMT
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Thanks for the explanation Thomas...

Jitender