
Subject: Re: Row Wise Sum

Posted by [nbehrnd](#) on Tue, 13 Jun 2023 18:49:47 GMT

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Dear Angus,

to answer the first question, you need a placeholder which either returns `0` (if there is nothing in the cell), or the value of the cell (if the cell contains an entry acceptable for an addition); `replaceempty` is suitable here. For the second question, you already tap against a good door; you now need to know how to negate a Boolean in DataWarrior's syntax.

For the purpose of illustration, I attach a minimal working example below. Departing from a small library of random molecules, DataWarrior computes the number of H-Donors and H-Acceptors. Manually added -- leaving some gaps is intentional -- two additional columns with manual entries, `counter_a` and `counter_b`. The `special_sum` then

```
HAcceptors + HDonors + replaceempty(counter_a, 0) + replaceempty(counter_b, 0)
```

either adds either the results of DataWarrior's intrinsic functions plus the zeroes, or the values of the additional columns. To count the the non-empty columns `!` offers to define

```
!isempty(HAcceptors) + !isempty(HDonors) + !isempty(counter_a) + !isempty(counter_b)
```

You can access, adjust and update the equations in question in the header cell of the corresponding column 7 and 8 (clique with the right mouse button).

With regards,

Norwid

File Attachments

1) [2023-06-13_Random_Molecules.dwar](#), downloaded 484 times
