Subject: Where do pKa values in pKaInWater.dwar come from ?
Posted by DrFunkenstein on Wed, 17 May 2017 15:42:09 GMT
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Hi,

7913 pKa values are provided in the pKaInWater.dwar file (thank you!!!). I'm wondering where these values came from? Literature? In-house experiments?

Thanks!
DrFunkenstein

Subject: Re: Where do pKa values in pKaInWater.dwar come from ?
Posted by thomas on Sat, 27 May 2017 22:30:18 GMT
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this is an old dataset that was originally compiled from the literature and hand-curated such that the structures represent the correct protonation state. Unluckily the original paper reference got lost or was never collected.

Thomas

Subject: Re: Where do pKa values in pKaInWater.dwar come from ?
Posted by chem95 on Tue, 19 Mar 2019 17:49:50 GMT
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Hi! I was wondering where I can find this pkaInWater dataset? I read about it in a paper but cannot locate it on the website.

Thanks so much

Subject: Re: Where do pKa values in pKaInWater.dwar come from ?
Posted by thomas on Wed, 20 Mar 2019 22:14:55 GMT
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it is part of the DataWarrior installation. You find it in the installation folder in the 'reference' folder. On Linux the instalation folder would be /opt/datawarrior, on Windows it is C:/Program Files/DataWarrior.

Thomas

Subject: Re: Where do pKa values in pKaInWater.dwar come from ?
Posted by chem95 on Thu, 21 Mar 2019 21:28:36 GMT
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Thank you for such a quick and helpful reply!

Within the dataset I see some identifiers about the molecule such as the "FragFp" and the "Structure". Is there a good way to convert one of these values into a SMILES string so that I can understand the molecules that correspond to these pKa measurements?

Subject: Re: Where do pKa values in pKaInWater.dwar come from ?
Posted by thomas on Sun, 24 Mar 2019 21:42:12 GMT
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you can open the dataset in DataWarrior and may generate SMILES, export as SD-File or as text file containing the SMILES, if you want.