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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

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