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?