Measurement of acidity constants for compounds SAMPL8-1, SAMPL8-2, SAMPL8-5, and SAMPL8-22

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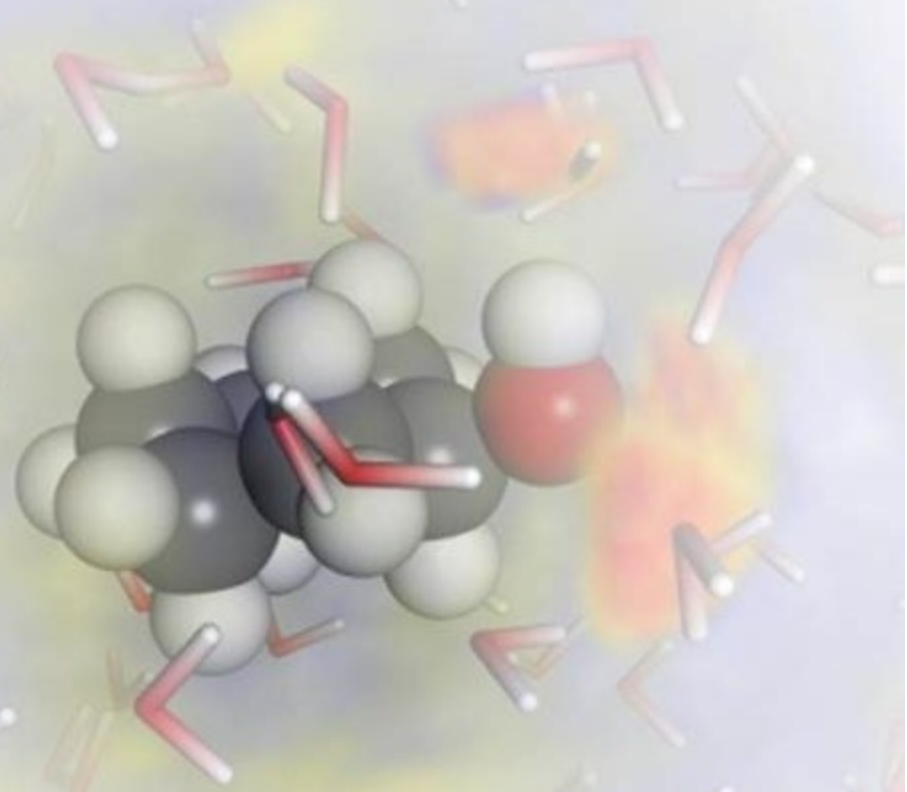
Measurements

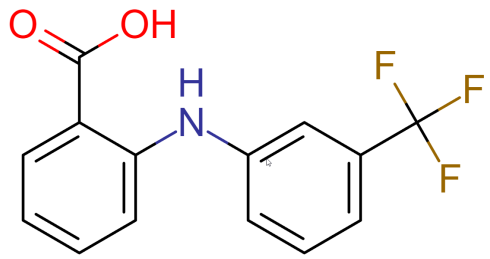
- Juliana Gretz
- Paul Czodrowski

Calculations / technical support

- Nicolas Tielker
- Stefan M. Kast

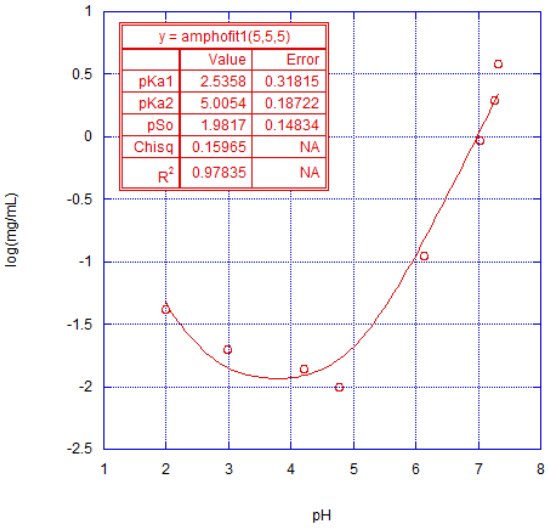


SAMPL8-1



original data

Predicted pK_a	3.88[1]
Experimental pK_a	2.54, 5.01[2]

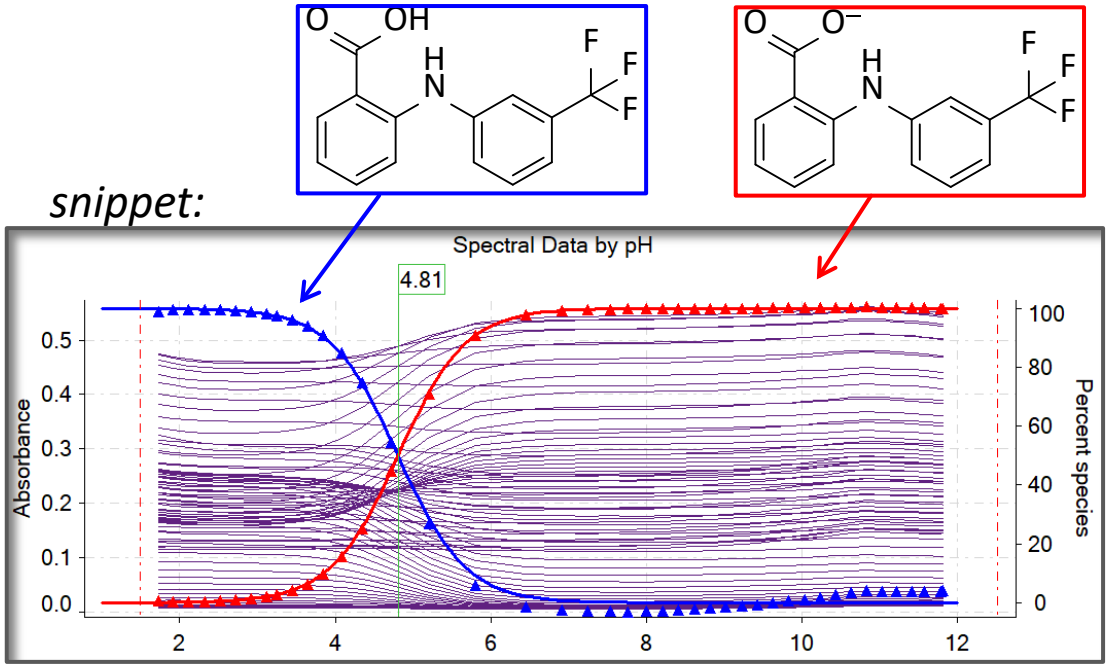


SiriusT3 Measurements

- Three measurements for each sample
- Three samples with different methanol concentrations
- Yasuda-Shedlovsky extrapolation
- Most likely microstates as predicted by EC-RISM

→ pK_a = **3.99 ± 0.07**

snippet:

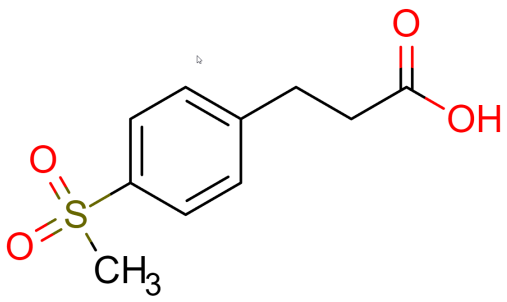


[1] ChemAxon JChem software with the pKa Plugin, ChemAxon, Budapest, Hungary

[2] M. N. Bahr, A. Nandkeolyar, J. K. Kenna, N. Nevins, L. Da Vìa, M. Işık, J. D. Chodera, D. L. Mobley, *J. Comput. Aided Mol. Des.*, **35**, 1141-1155, 2021

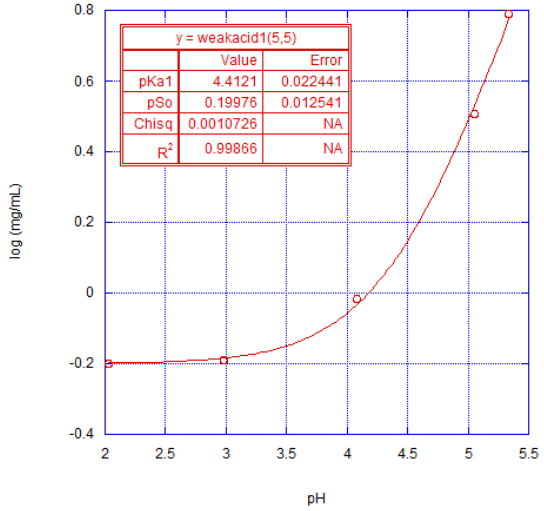
https://github.com/samplchallenges/SAMPL8/blob/master/physical_properties/experimental_data/SAMPL8%20Final%20Readout_pH-Solubility%20Pub.pptx

SAMPL8-2



original data

Predicted pK_a	3.49[1]
Experimental pK_a	4.41[2]

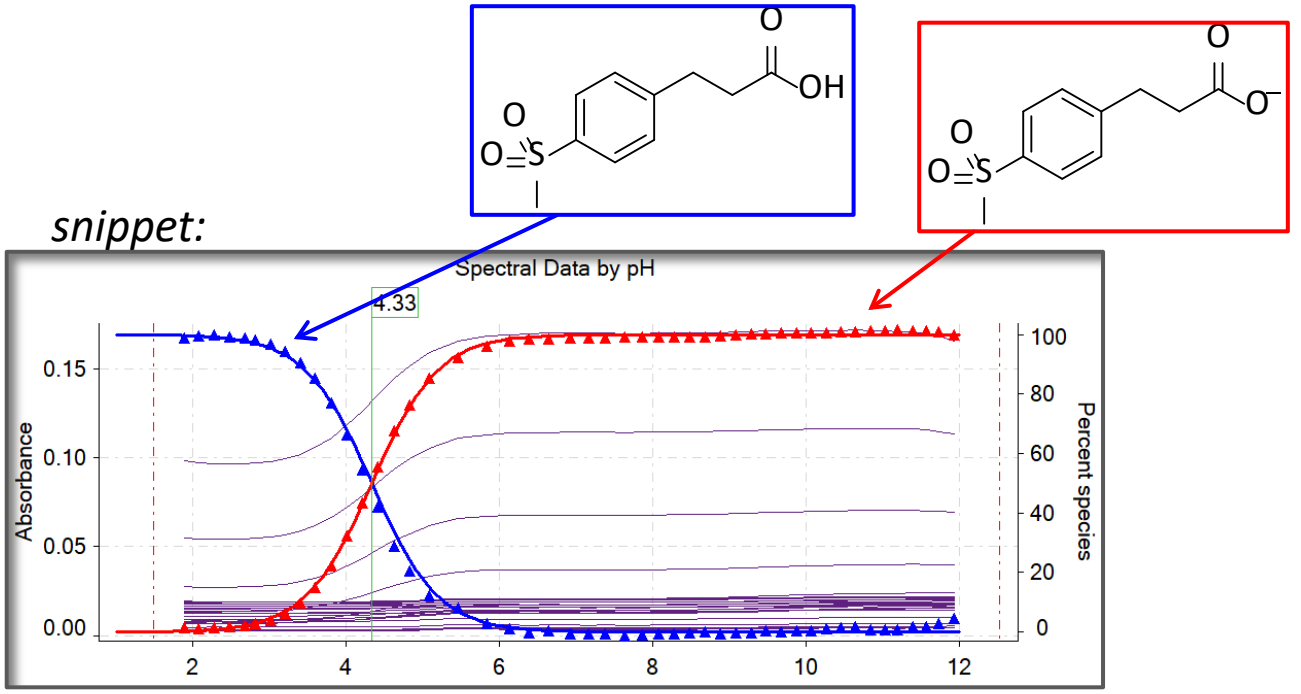


SiriusT3 Measurements

- Three measurements for each sample
- Three samples in total
- Most likely microstates as predicted by EC-RISM

→ pK_a = **4.50 ± 0.07**

snippet:



[1] ChemAxon JChem software with the pKa Plugin, ChemAxon, Budapest, Hungary

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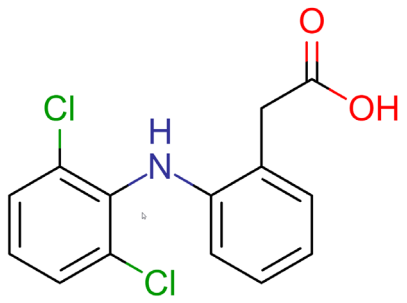
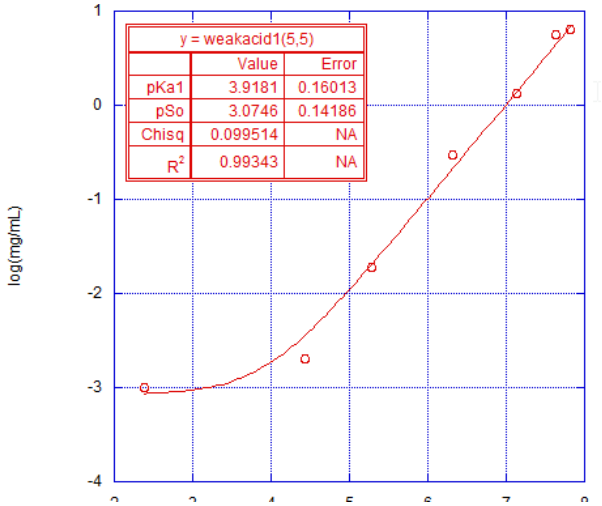
SAMPL8-5



original data

Predicted pK_a	4.00[1]
Experimental pK_a	3.92[2]

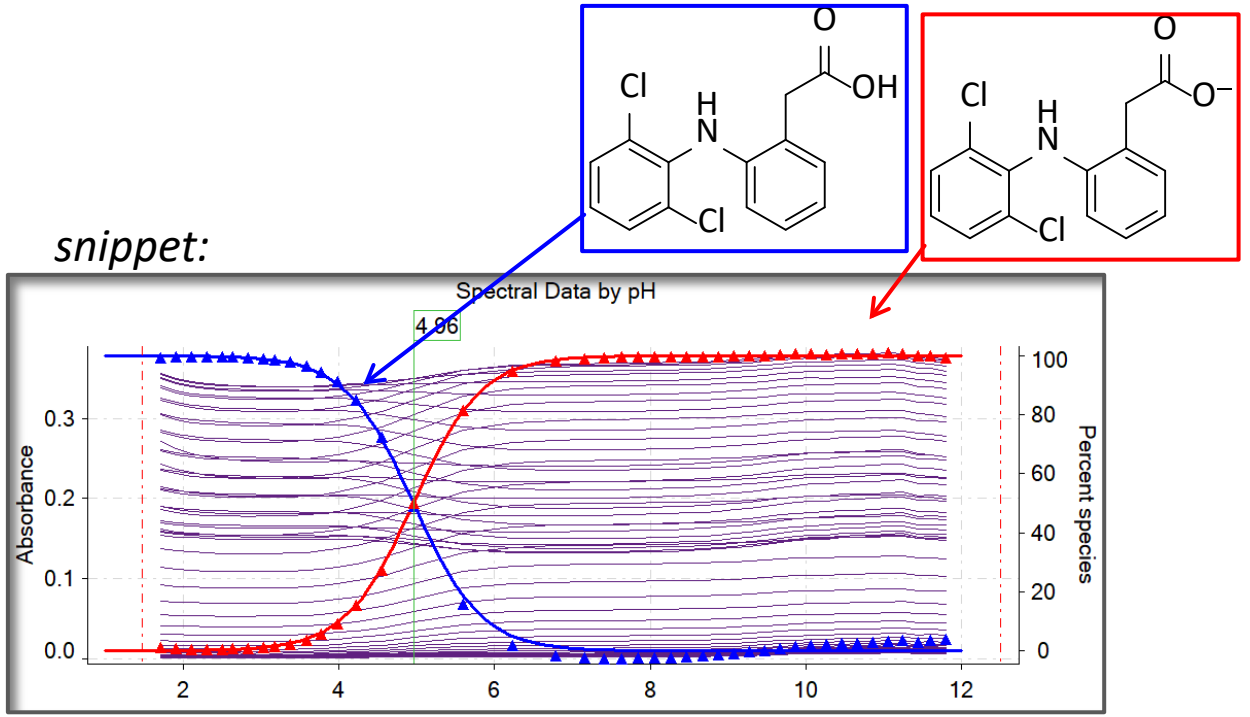


SiriusT3 Measurements

- Three measurements for each sample
- Three samples with different methanol concentrations
- Yasuda-Shedlovsky extrapolation
- Most likely microstates as predicted by EC-RISM

→ pK_a = **4.23 ± 0.07**

snippet:



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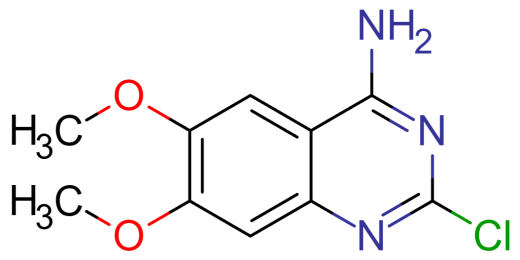
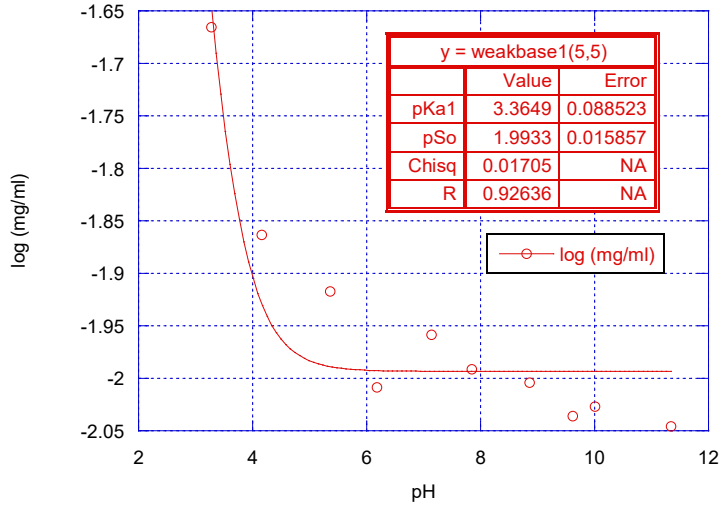
SAMPL8-22



original data

Predicted pK_a	2.94[1]
Experimental pK_a	3.36[2]

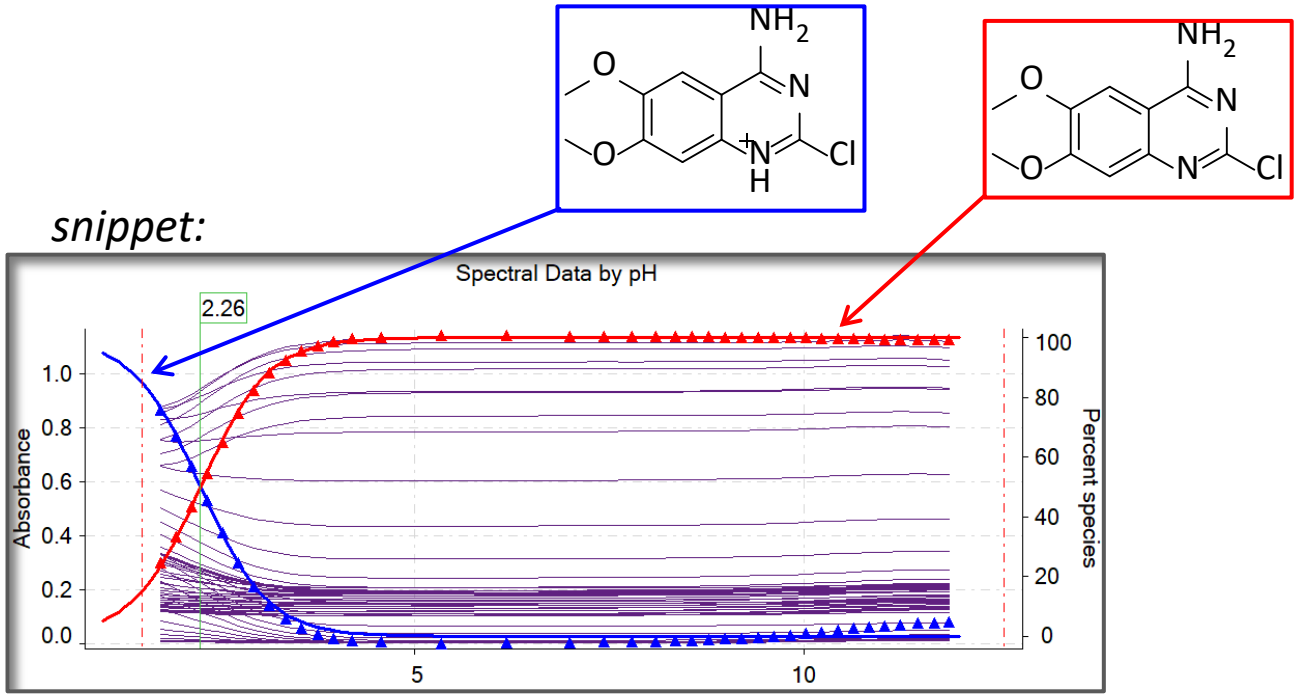


SiriusT3 Measurements

- Three measurements for each sample
- Three samples with different methanol concentrations
- Yasuda-Shedlovsky extrapolation
- Most likely microstates as predicted by EC-RISM

→ pK_a = **2.57 ± 0.09**

snippet:



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