



Yasuda-Shedlovsky Result

Sample name: **CS000270**
Assay name: **Fast UV psKa**
Assay ID: **11I-09012**
Filename: **E:\T3 DATA\1109\11I-09012_CS000270_Fast UV psKa.t3r**

Experiment start time: **09/09/2011 14:10:38**
Analyst:
Instrument ID: **T311042**

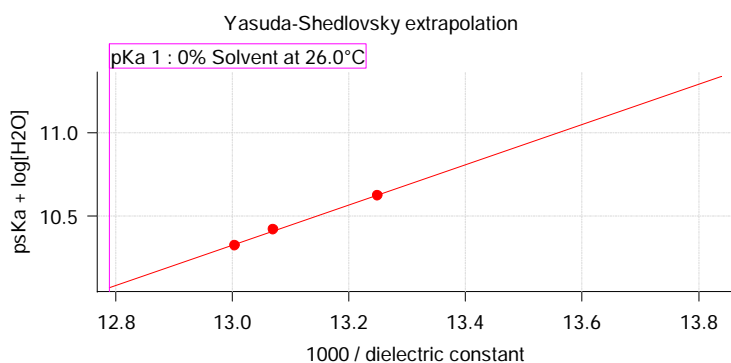
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	8.32	±0.02	-5.44	1212.5200	0.9976	0.208 M	26.0°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H ₂ O]	Ionic strength	Temperature	psKa 1
11I-09012 Points 107 to 160	23.64 %	Up	UV-metric pKa	76.9	43.2 M	0.213 M	26.3°C	✓ 8.69
11I-09012 Points 54 to 106	31.93 %	Up	UV-metric pKa	76.5	38.8 M	0.210 M	25.9°C	✓ 8.83
11I-09012 Points 3 to 53	42.60 %	Up	UV-metric pKa	75.5	33.0 M	0.202 M	25.8°C	✓ 9.10

Graphs

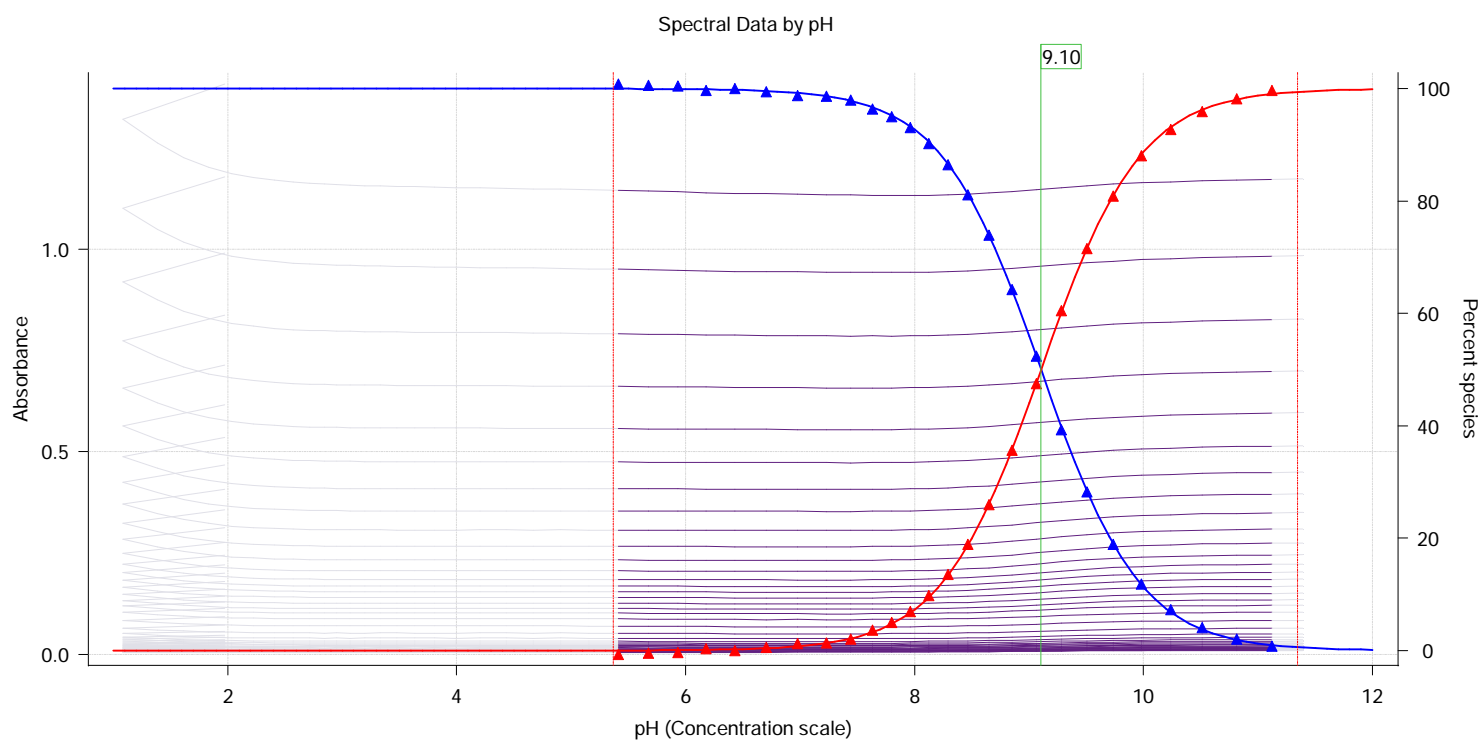
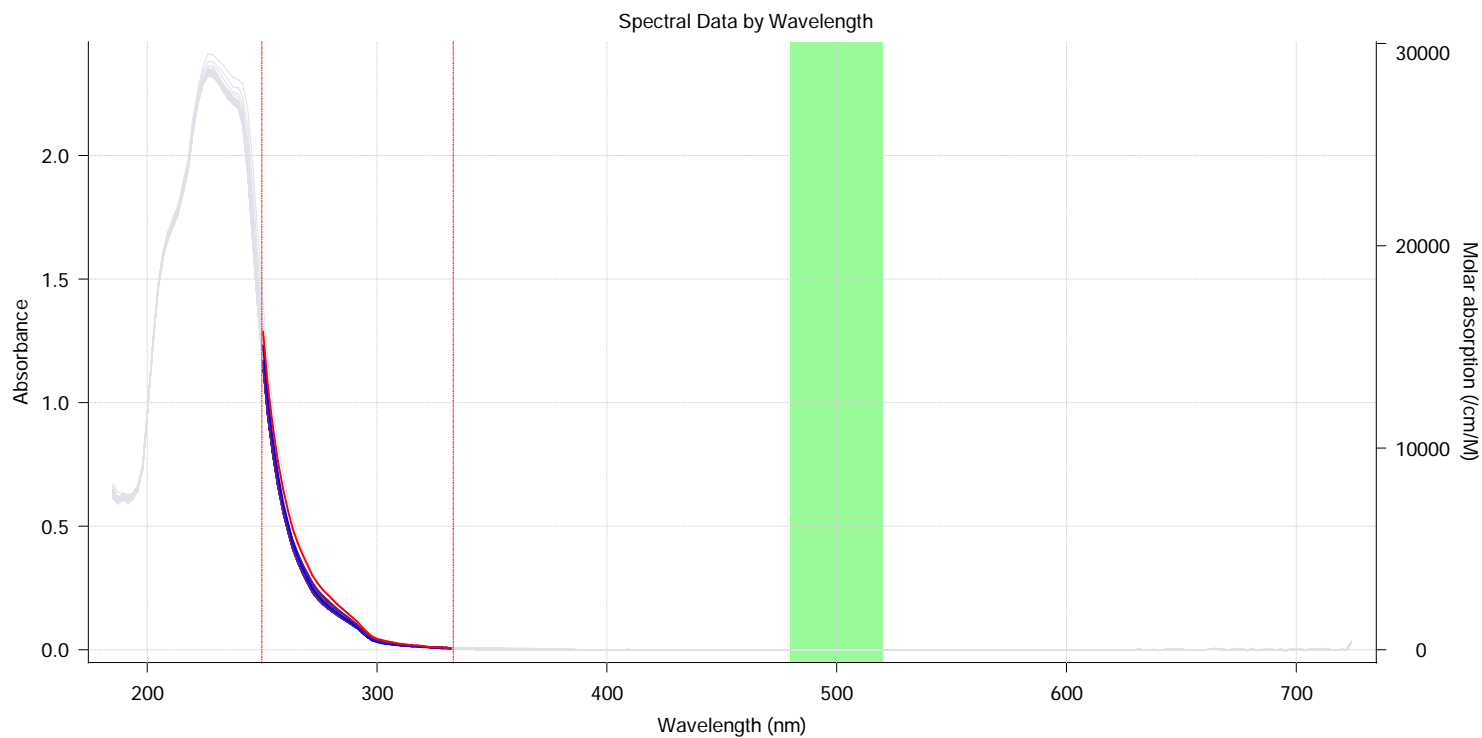


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Fast UV psKa Titration 1 of 3 11I-09012 Points 3 to 53

Graphs

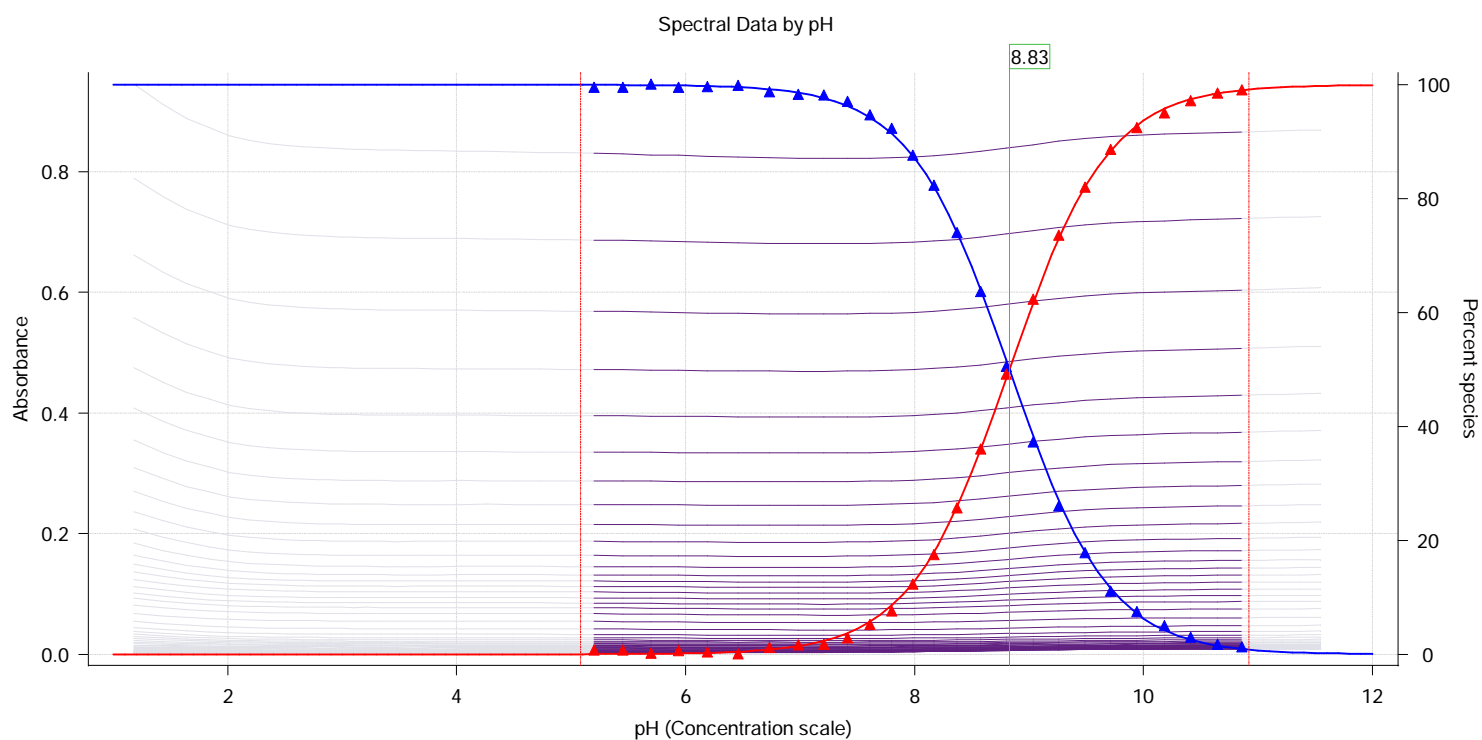
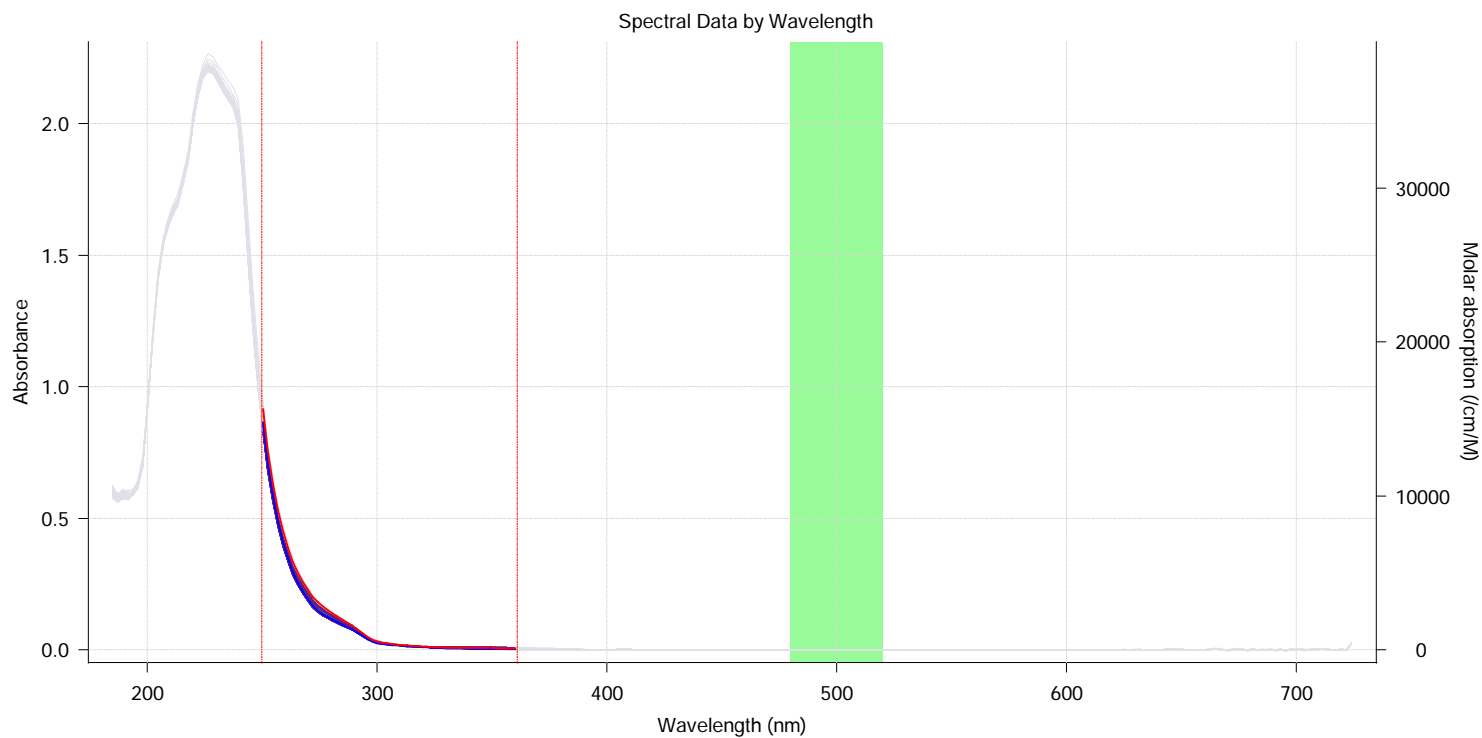


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Fast UV psKa Titration 2 of 3 11I-09012 Points 54 to 106

Graphs

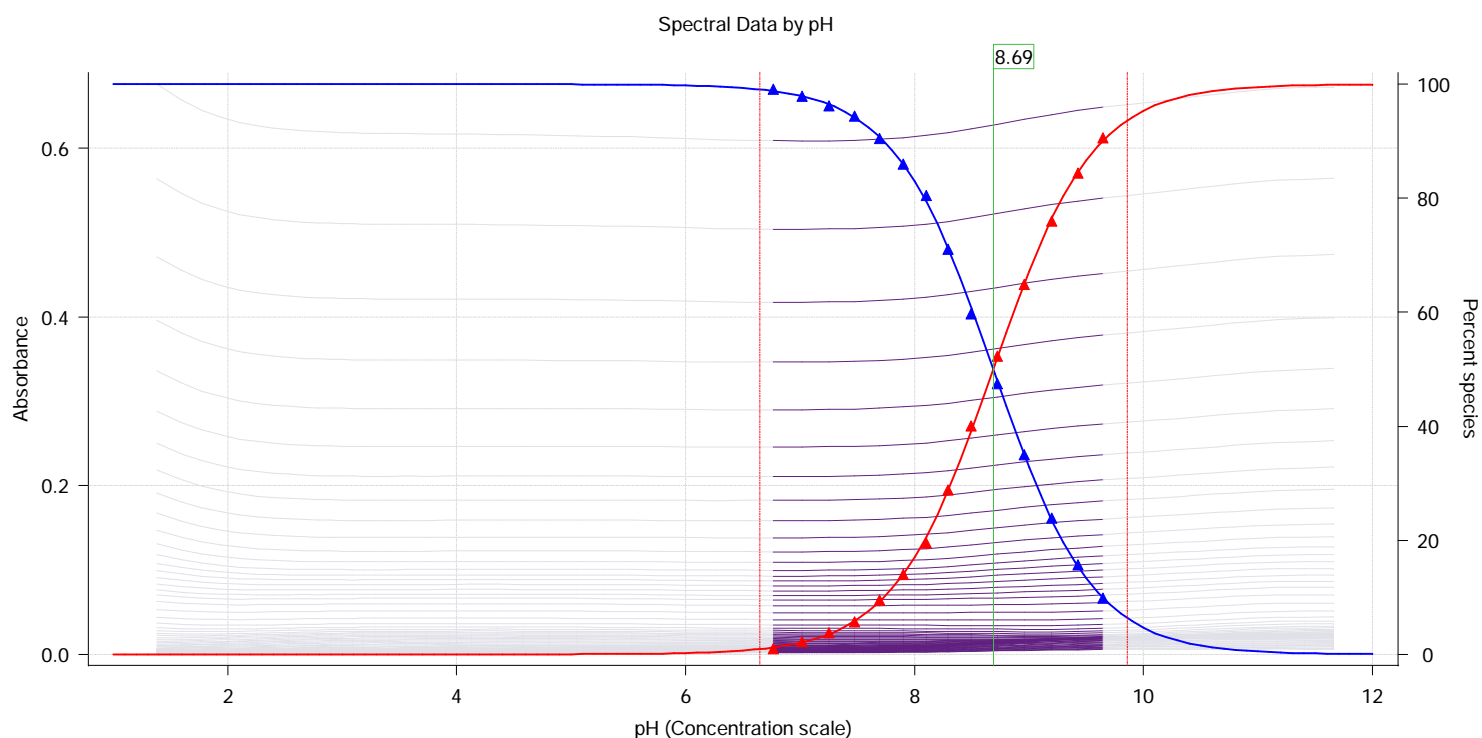
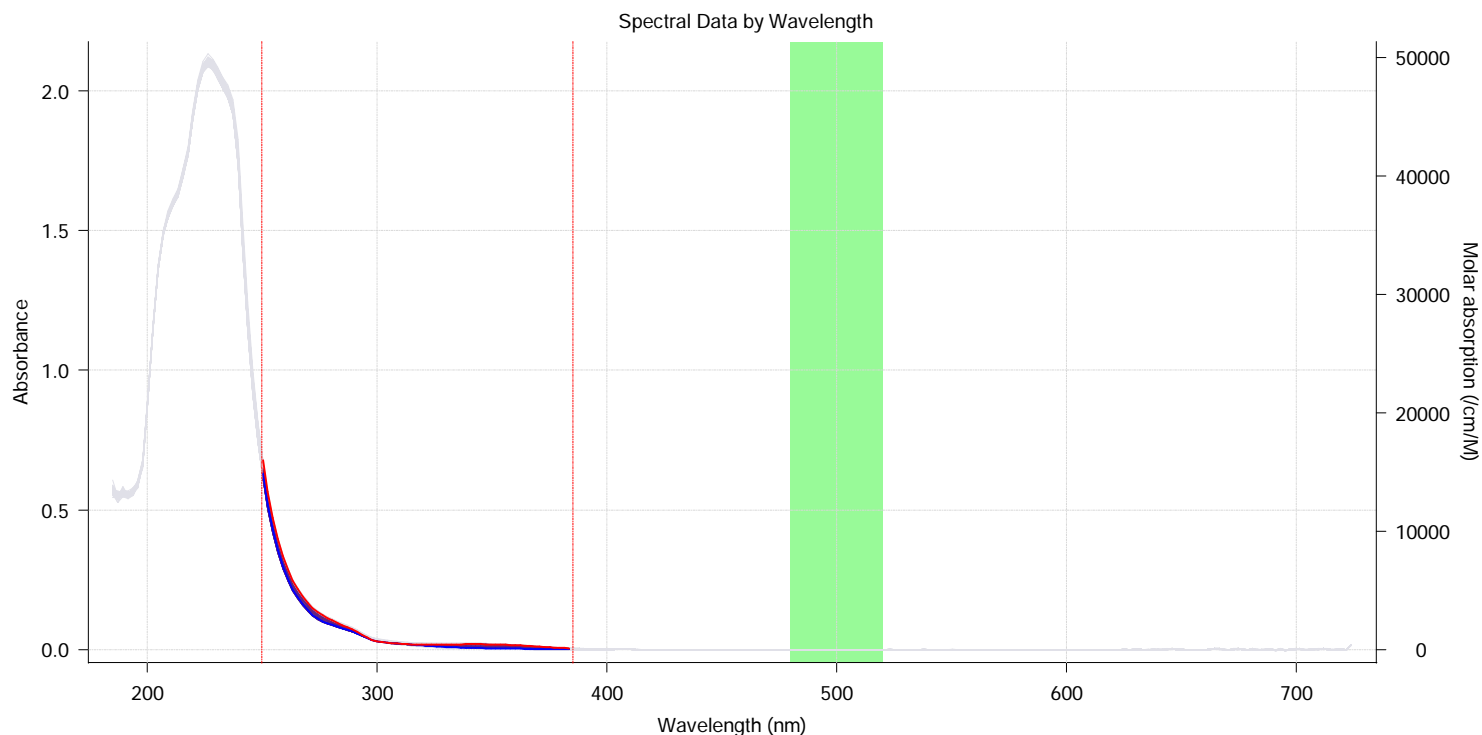


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Experiment start time: **09/09/2011 14:10:38**
 Analyst:
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Fast UV psKa Titration 3 of 3 11I-09012 Points 107 to 160

Graphs





Assay model

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Analyst:
Instrument ID: **T311042**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000270		
Sample by	Volume		
Sample volume	0.0150 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	09/09/2011 13:44:20	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	324.64		
Individual pKa ionic environments	No		
Number of pKas	1	09/09/2011 13:44:20	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Sample is a	Base	09/09/2011 13:44:20	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	4.00	09/09/2011 13:44:20	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logp (XH +)	-10.00	09/09/2011 13:44:20	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logP (neutral X)	-10.00	09/09/2011 13:44:20	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
