



## Yasuda-Shedlovsky Result

Sample name: **CS000252**  
Assay name: **Fast UV psKa**  
Assay ID: **11I-09015**  
Filename: **E:\T3 DATA\1109\11I-09015\_CS000252\_Fast UV psKa.t3r**

Experiment start time: **09/09/2011 15:29:38**  
Analyst:  
Instrument ID: **T311042**

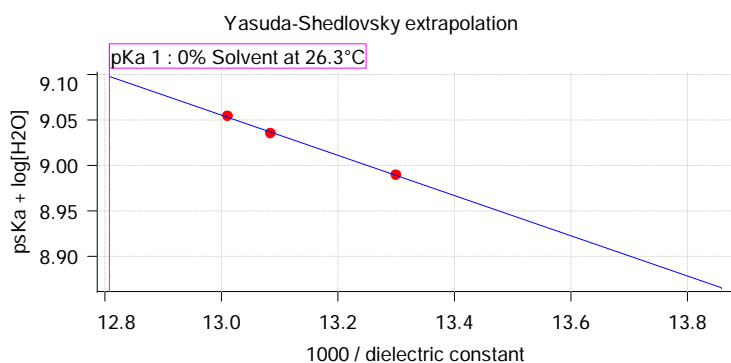
### Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R <sup>2</sup>	Ionic strength	Temperature
Yasuda-Shedlovsky	7.36	±0.00	11.93	-221.2748	0.9980	0.208 M	26.3°C

### Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H <sub>2</sub> O]	Ionic strength	Temperature	psKa 1
11I-09015 Points 107 to 160	23.59 %	Up	UV-metric pKa	76.9	43.2 M	0.212 M	26.4°C	✓ 7.42
11I-09015 Points 54 to 106	31.76 %	Up	UV-metric pKa	76.4	38.9 M	0.211 M	26.1°C	✓ 7.45
11I-09015 Points 3 to 53	43.37 %	Up	UV-metric pKa	75.2	32.6 M	0.201 M	26.4°C	✓ 7.48

### Graphs

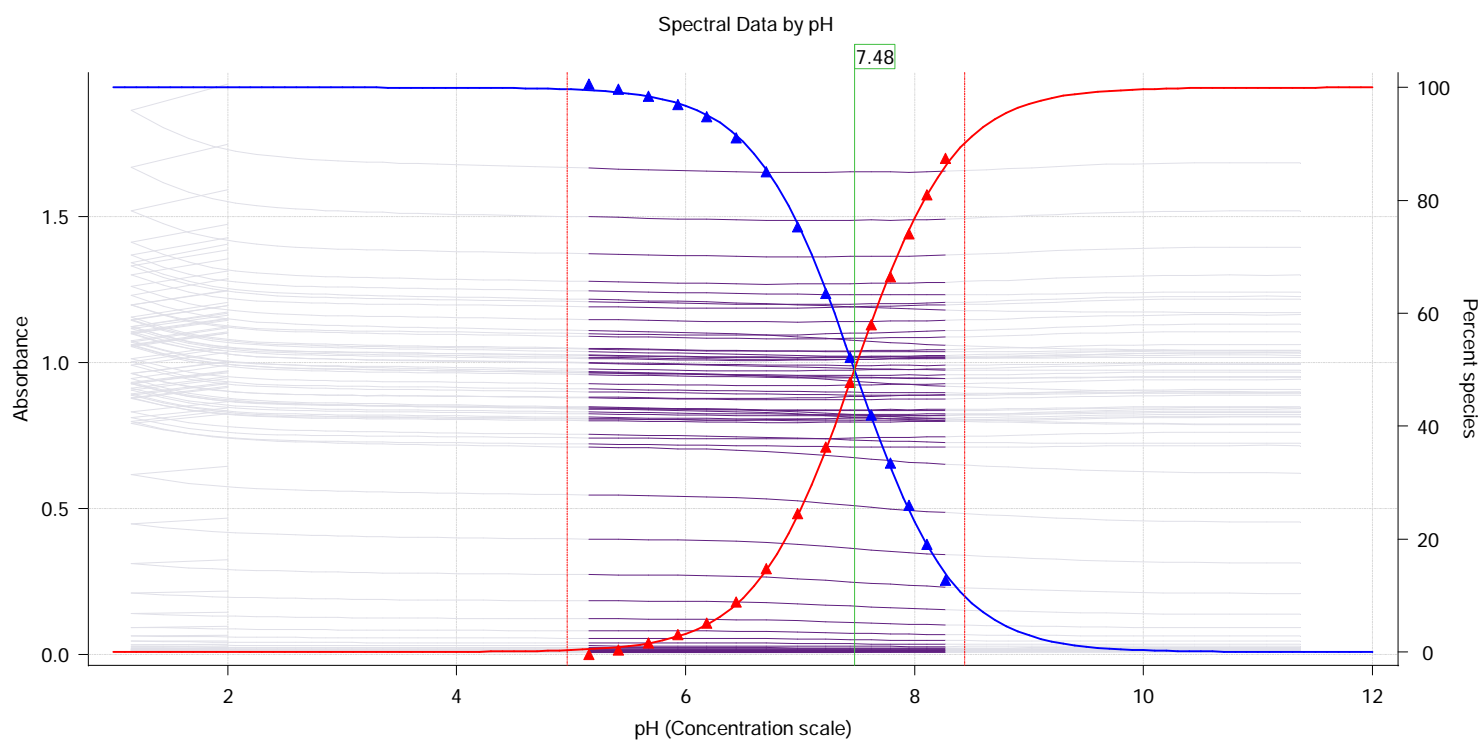
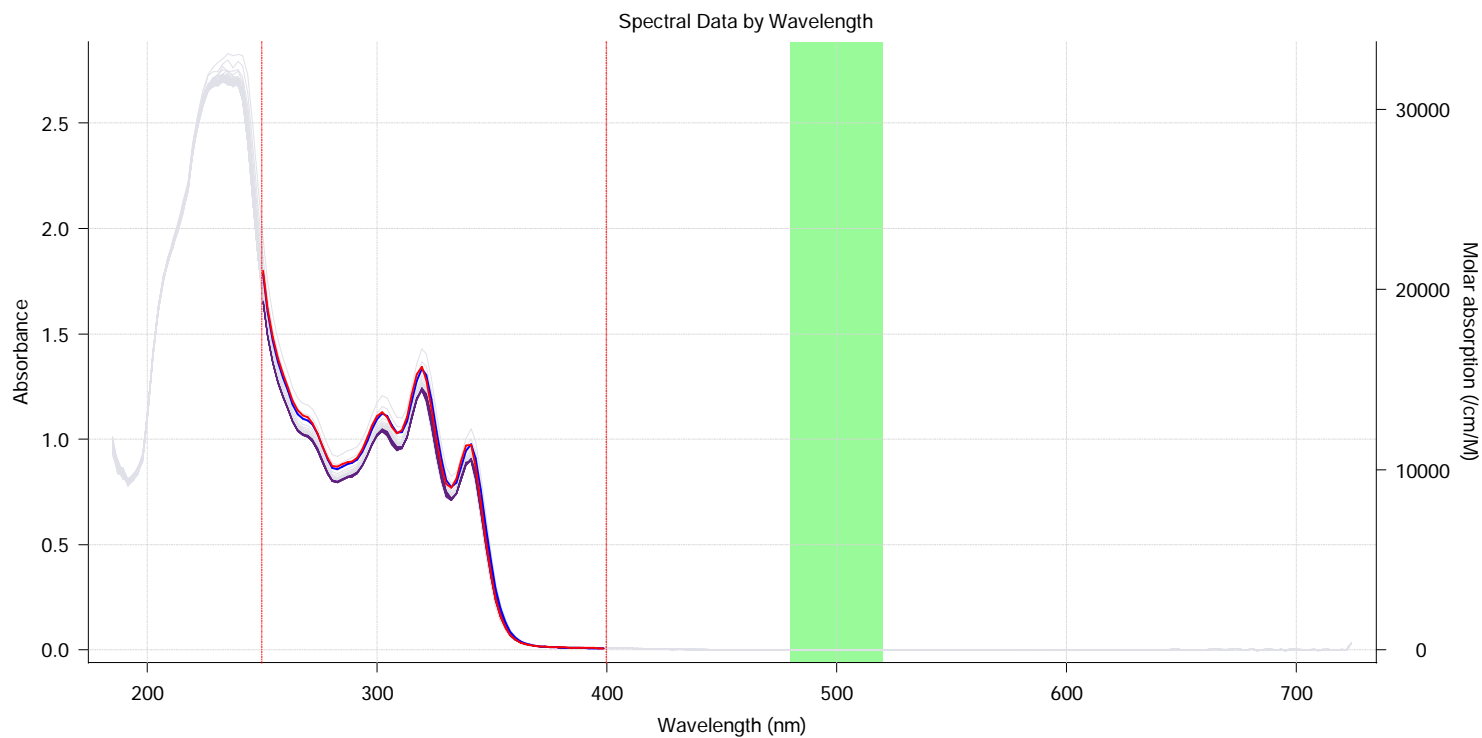


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## Fast UV psKa Titration 1 of 3 11I-09015 Points 3 to 53

### Graphs

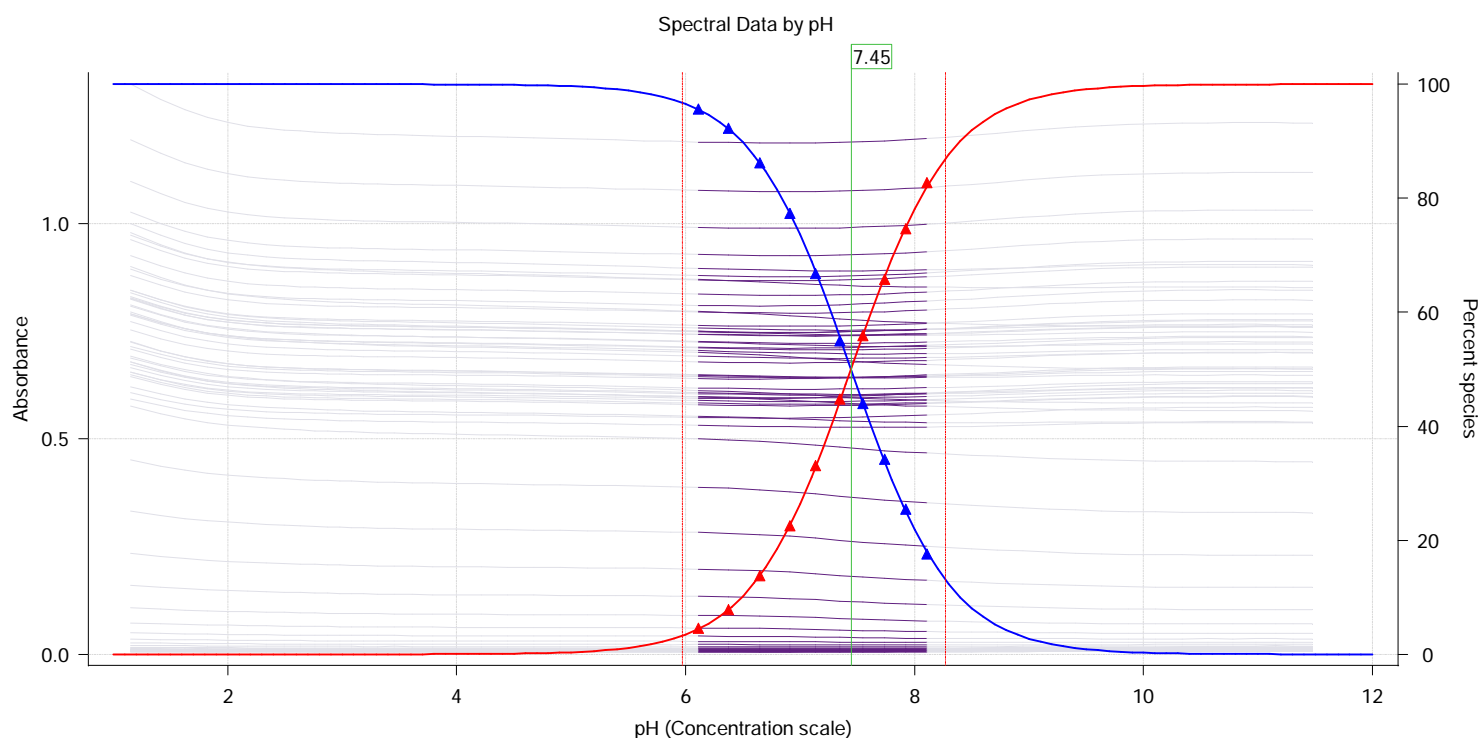
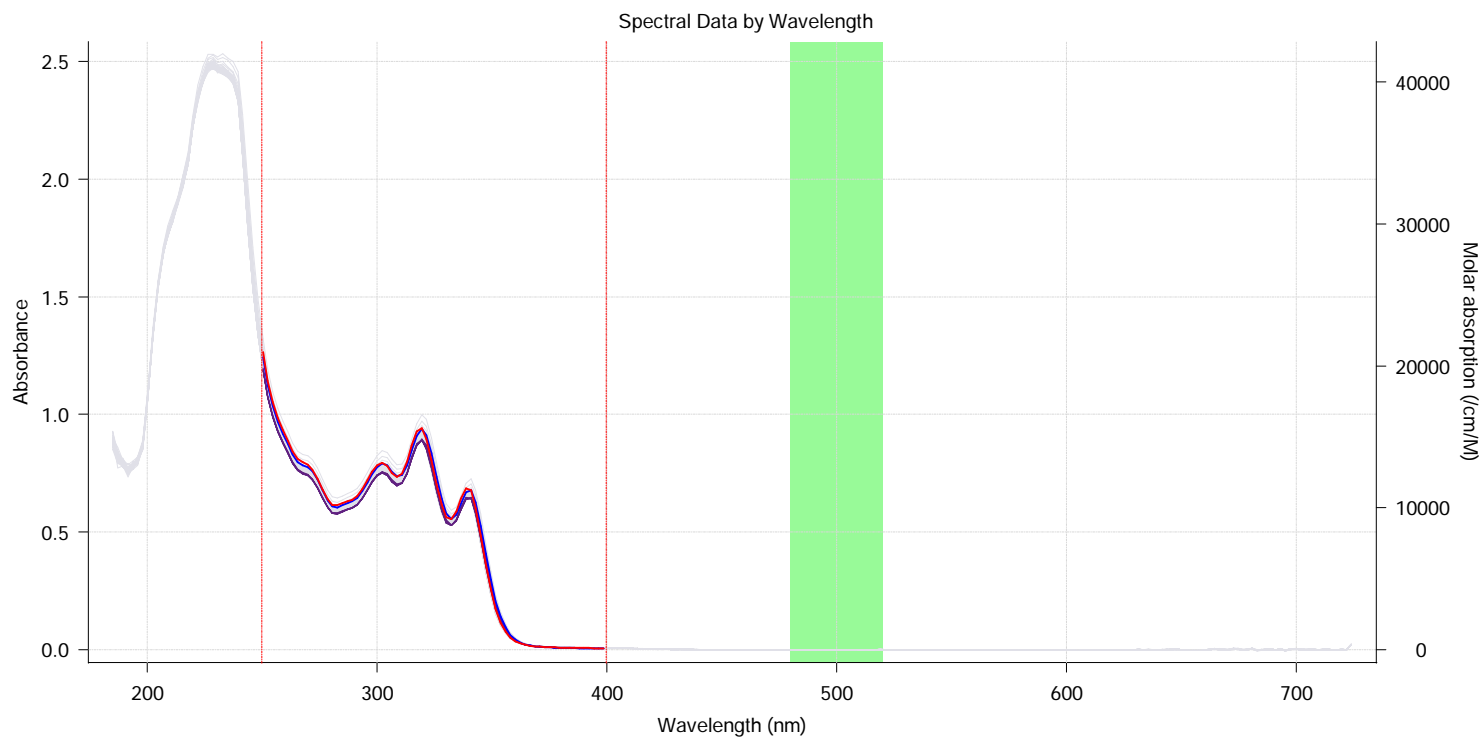


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## Fast UV psKa Titration 2 of 3 11I-09015 Points 54 to 106

### Graphs

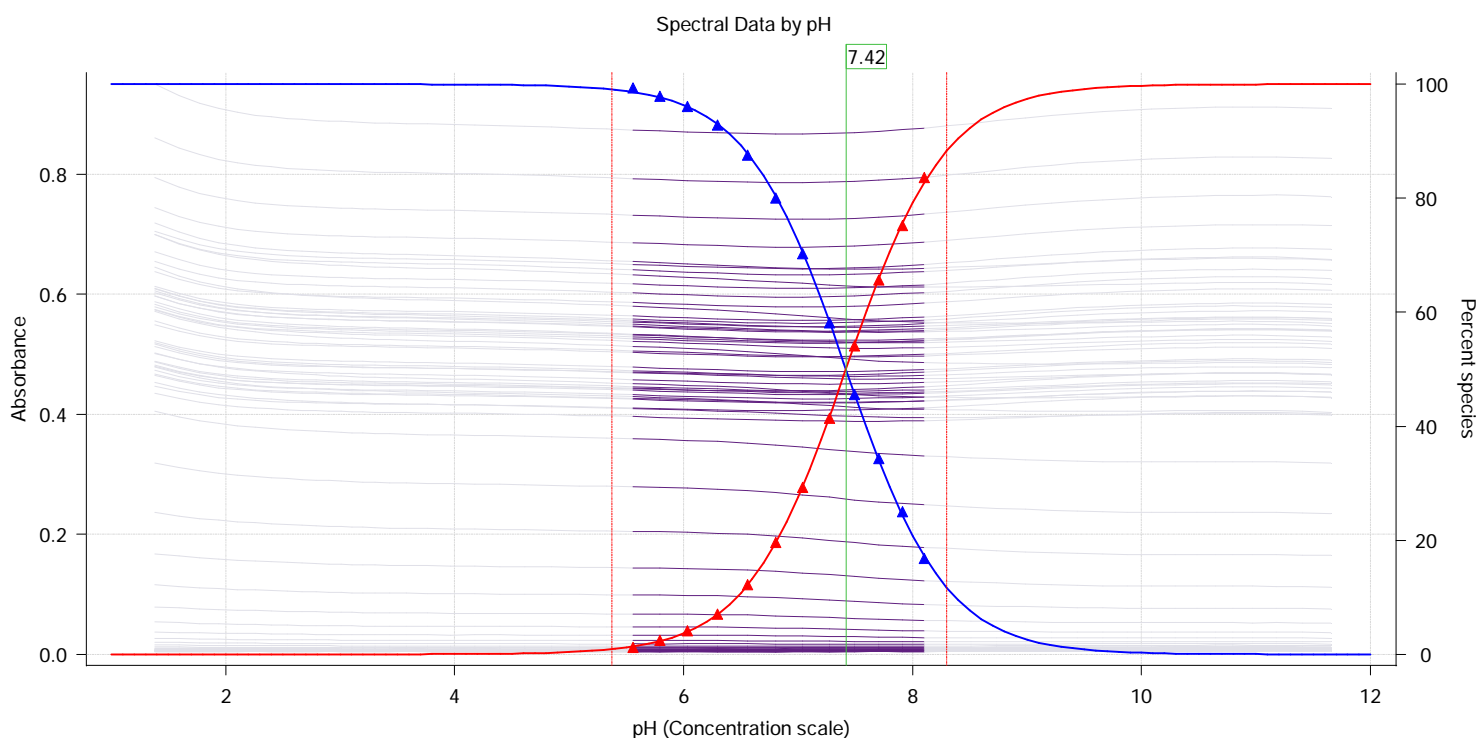
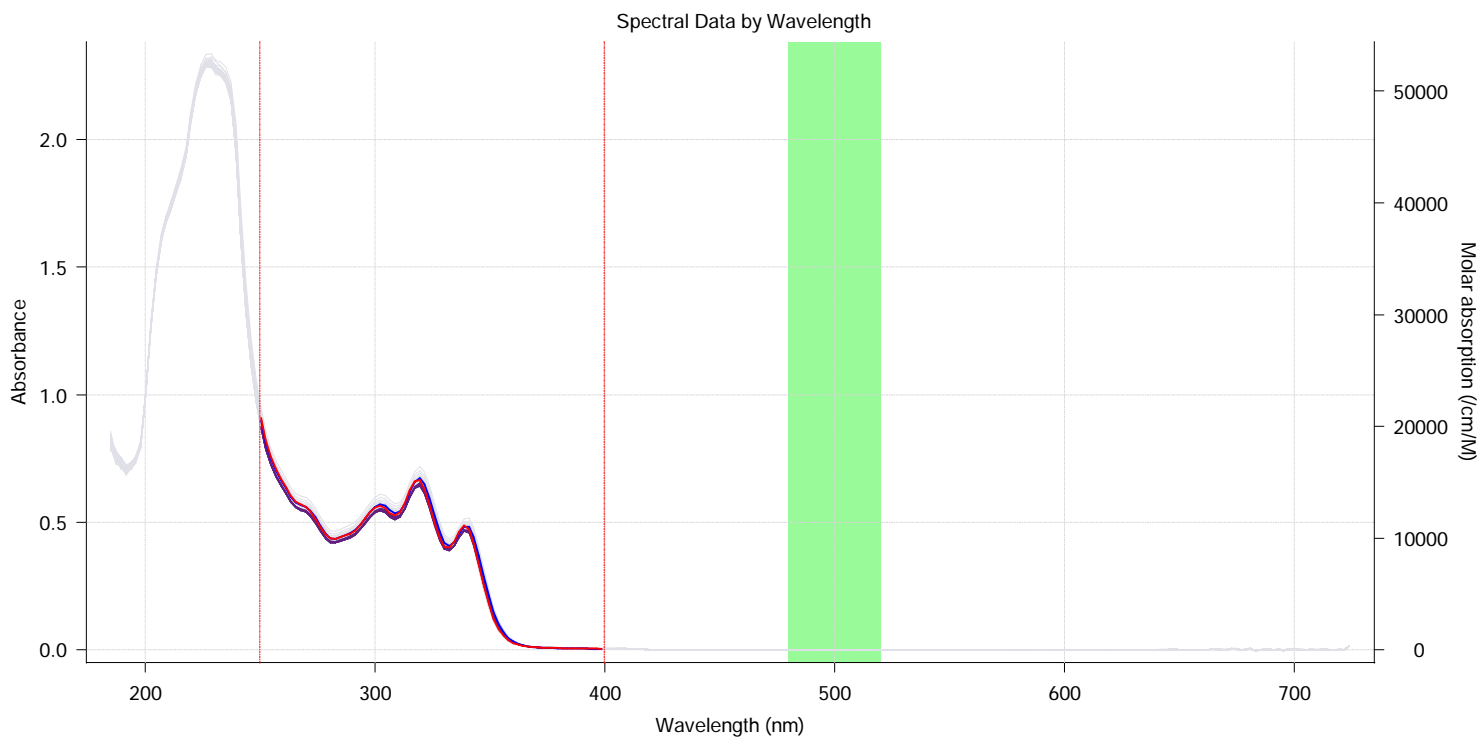


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Experiment start time: **09/09/2011 15:29:38**  
 Analyst:  
 Instrument ID: **T311042**

## Fast UV psKa Titration 3 of 3 11I-09015 Points 107 to 160

### Graphs





## Assay model

Sample name: **CS000252**  
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Filename: **E:\T3 DATA\1109\11I-09015\_CS000252\_Fast UV psKa.t3r**

Experiment start time: **09/09/2011 15:29:38**  
Analyst:  
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### Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000252		
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	347.37		
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

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