



Yasuda-Shedlovsky Result

Sample name: **CS000274**
Assay name: **Fast UV psKa**
Assay ID: **11I-02008**
Filename: **E:\T3 DATA\1109\11I-02008_CS000274_Fast UV psKa.t3r**

Experiment start time: **02/09/2011 11:24:38**
Analyst:
Instrument ID: **T311042**

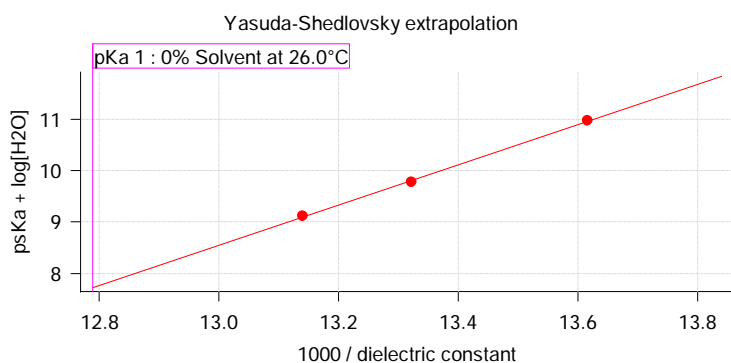
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	5.98	±0.06	-42.34	3914.2918	0.9994	0.195 M	26.0°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature	psKa 1
11I-02008 Points 89 to 129	36.96 %	Up	UV-metric pKa	76.1	36.1 M	0.196 M	25.8°C	✓ 7.56
11I-02008 Points 46 to 88	45.71 %	Up	UV-metric pKa	75.1	31.3 M	0.196 M	25.8°C	✓ 8.28
11I-02008 Points 3 to 45	54.21 %	Up	UV-metric pKa	73.4	26.6 M	0.192 M	26.4°C	✓ 9.54

Graphs

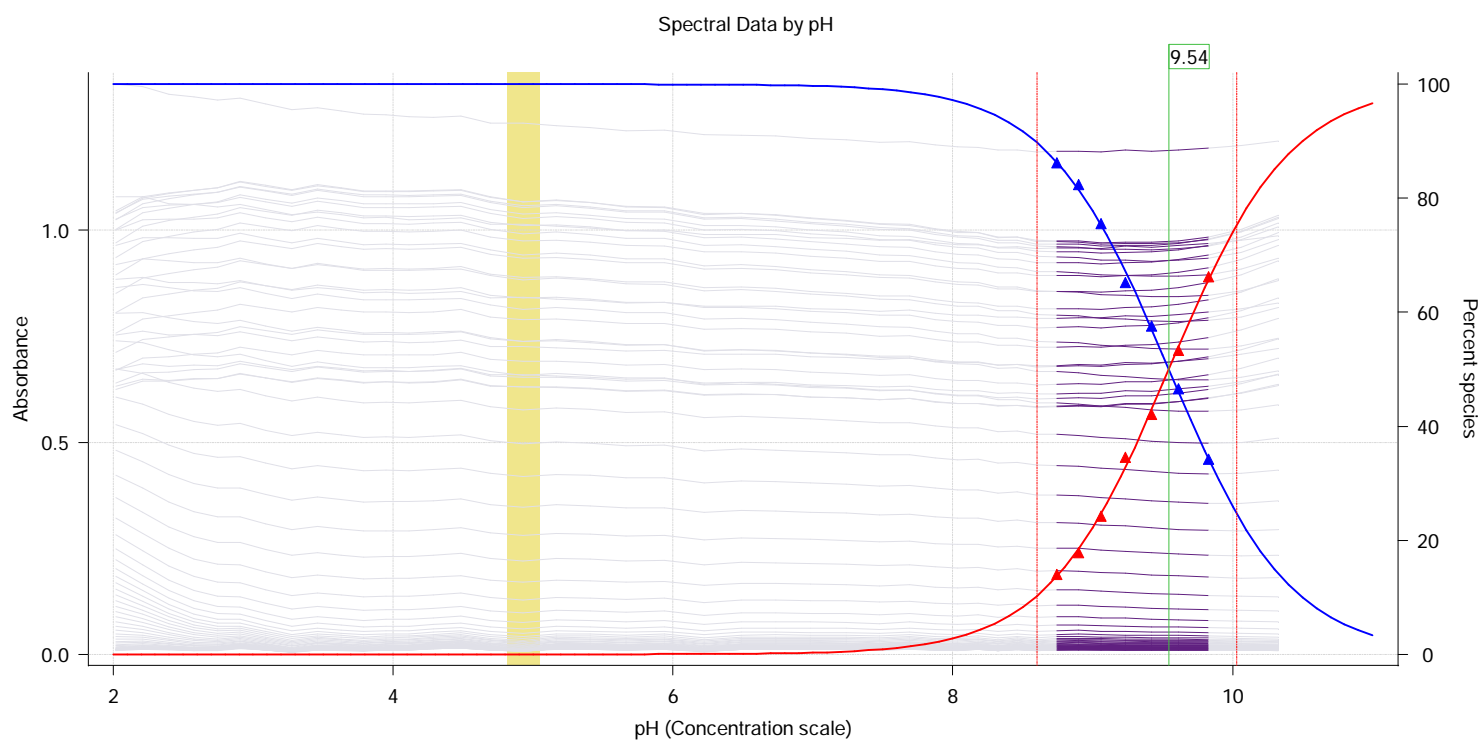
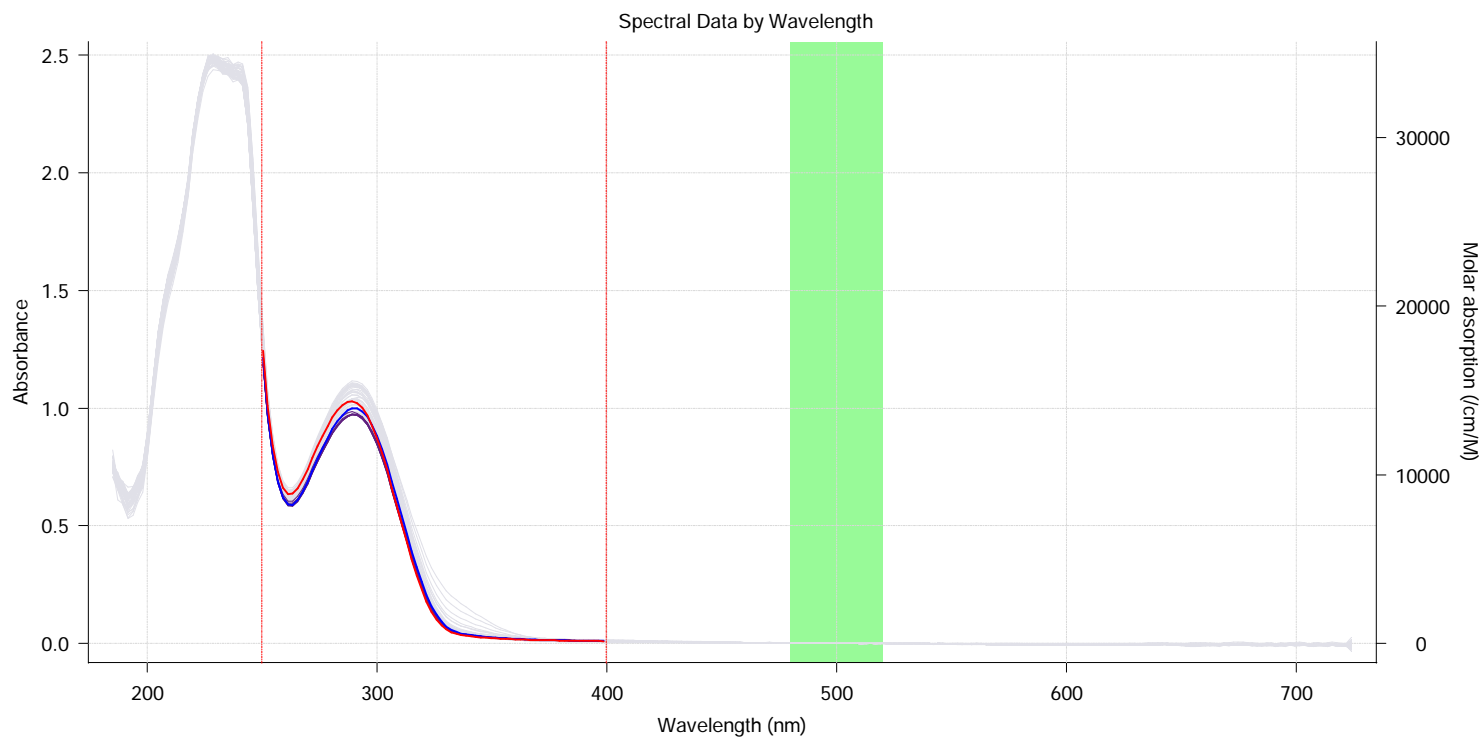


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Fast UV psKa Titration 1 of 3 11I-02008 Points 3 to 45

Graphs

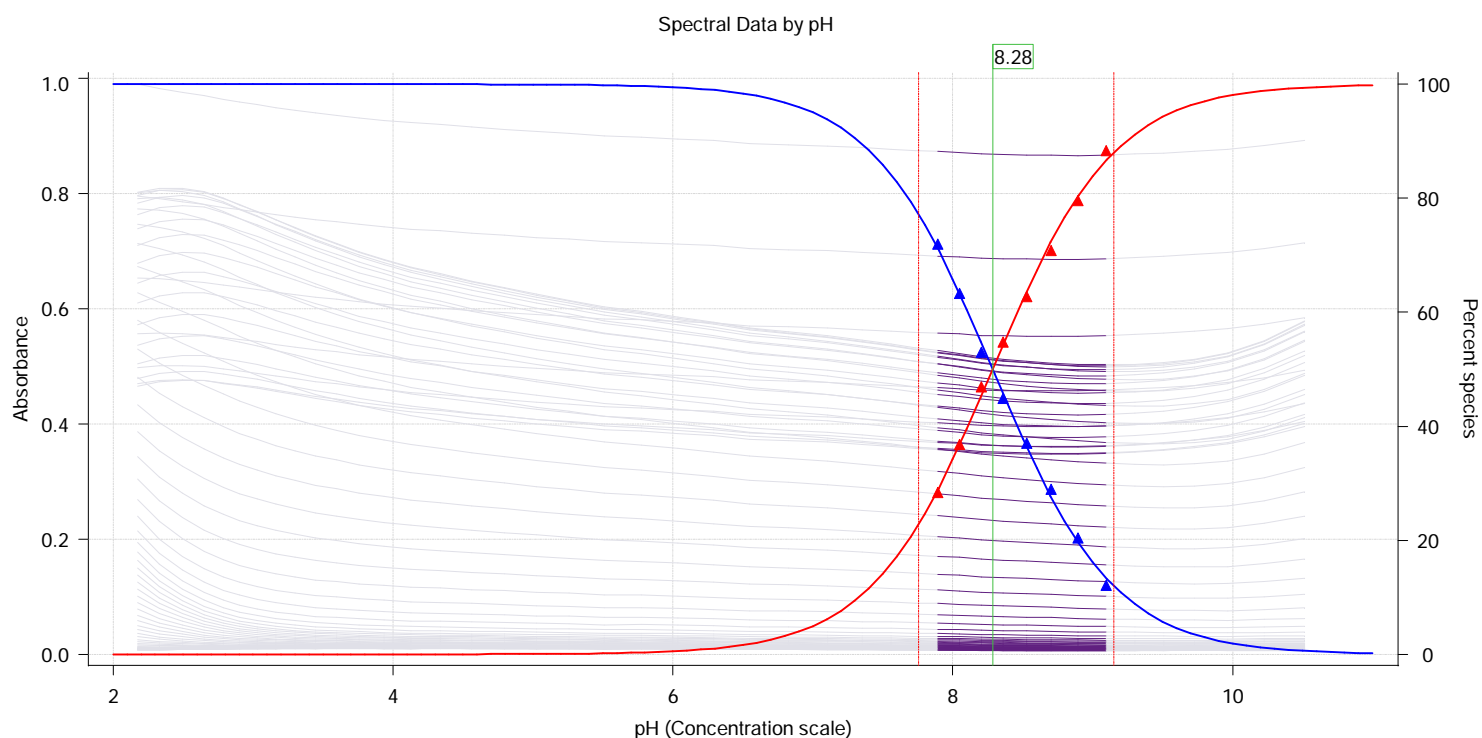
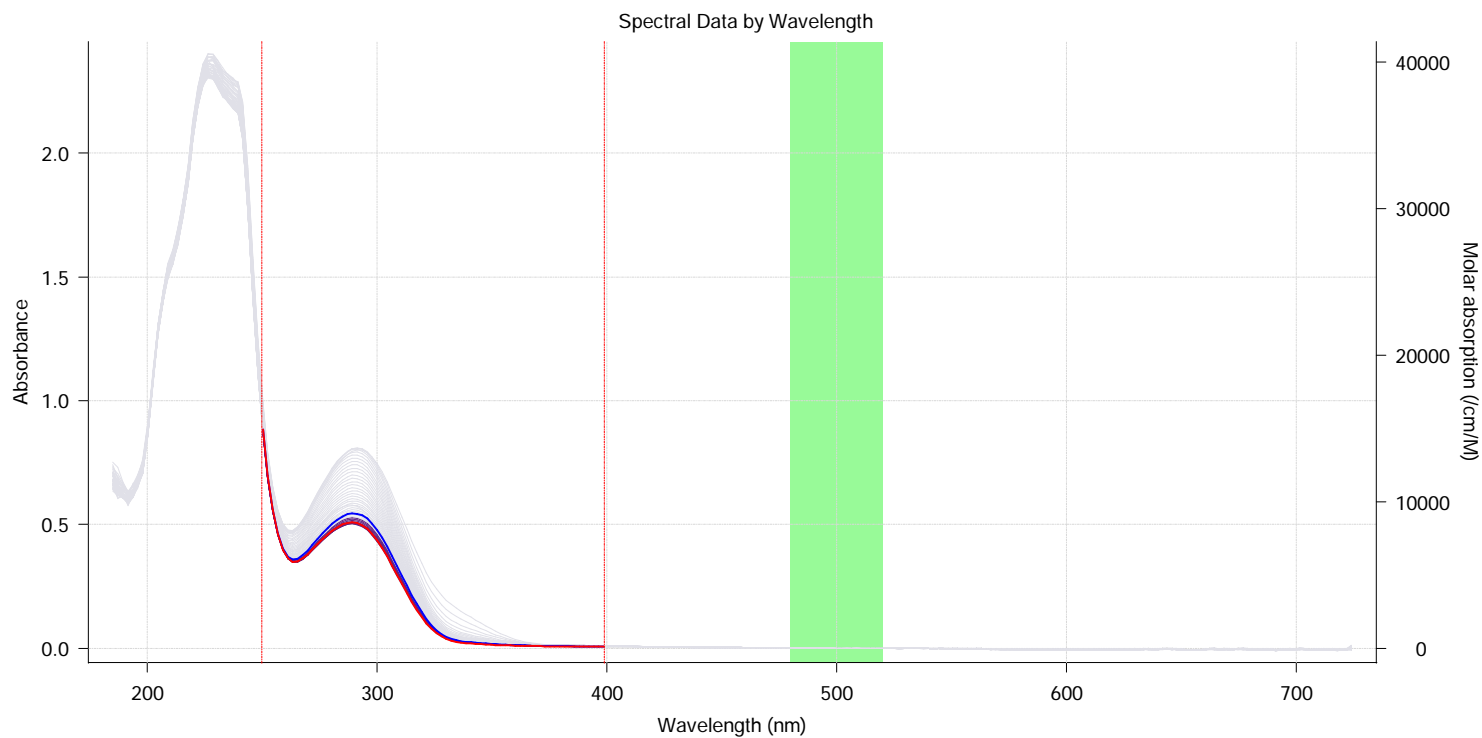


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Fast UV psKa Titration 2 of 3 11I-02008 Points 46 to 88

Graphs

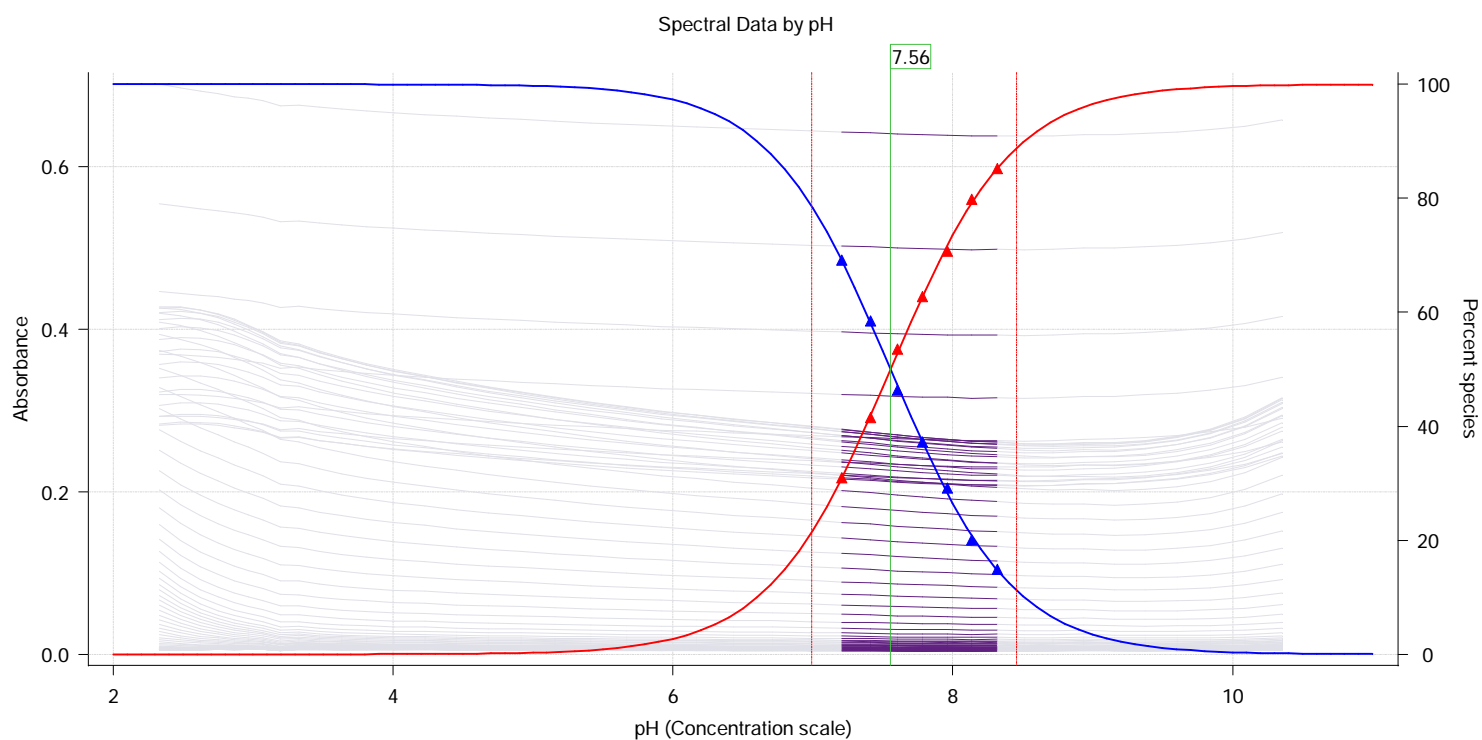
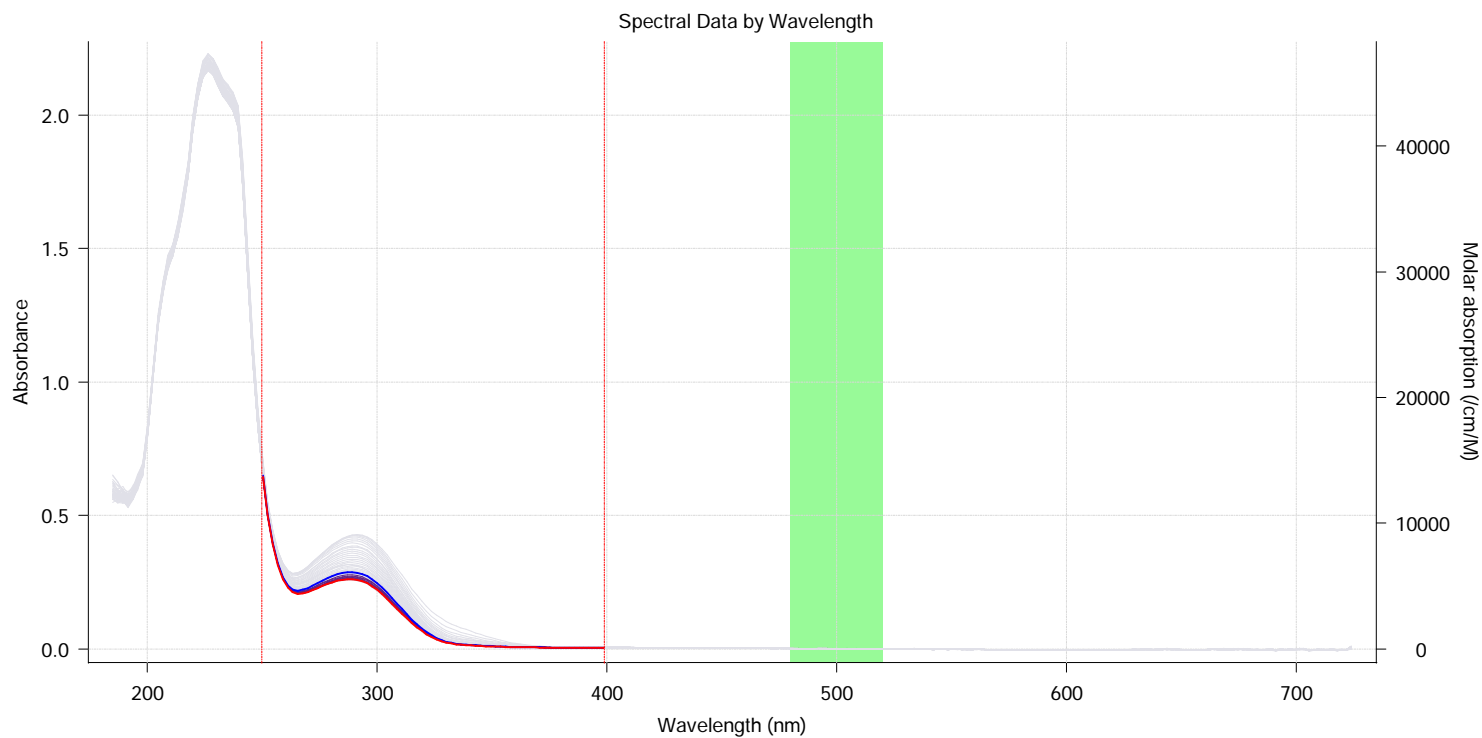


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Fast UV psKa Titration 3 of 3 11I-02008 Points 89 to 129

Graphs





Assay model

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Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000274		
Sample by	Volume		
Sample volume	0.0100 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	02/09/2011 10:09:27	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	324.37		
Individual pKa ionic environments	No		
Number of pKas	1	02/09/2011 10:09:27	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Sample is a	Base	02/09/2011 10:09:27	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	4.00	02/09/2011 10:09:27	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logp (XH +)	-10.00	02/09/2011 10:09:27	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logP (neutral X)	-10.00	02/09/2011 10:09:27	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
