



Yasuda-Shedlovsky Result

Sample name: **CS000243**
Assay name: **Fast UV psKa**
Assay ID: **11H-31014**
Filename: **E:\T3 DATA\1108\11H-31014_CS000243_Fast UV psKa.t3r**

Experiment start time: **31/08/2011 19:31:30**
Analyst:
Instrument ID: **T311042**

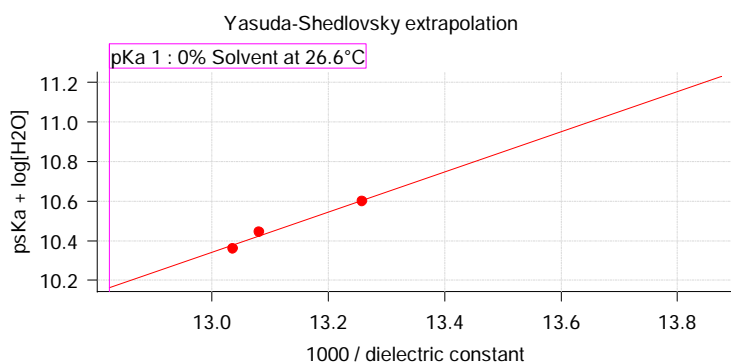
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	8.42	±0.05	-2.84	1013.7754	0.9745	0.211 M	26.6°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H ₂ O]	Ionic strength	Temperature	psKa 1
11H-31014 Points 105 to 154	23.08 %	Up	UV-metric pKa	76.7	43.4 M	0.215 M	26.9°C	✓ 8.72
11H-31014 Points 54 to 104	31.04 %	Up	UV-metric pKa	76.4	39.3 M	0.214 M	26.2°C	✓ 8.85
11H-31014 Points 3 to 53	40.81 %	Up	UV-metric pKa	75.4	34.0 M	0.204 M	26.6°C	✓ 9.07

Graphs

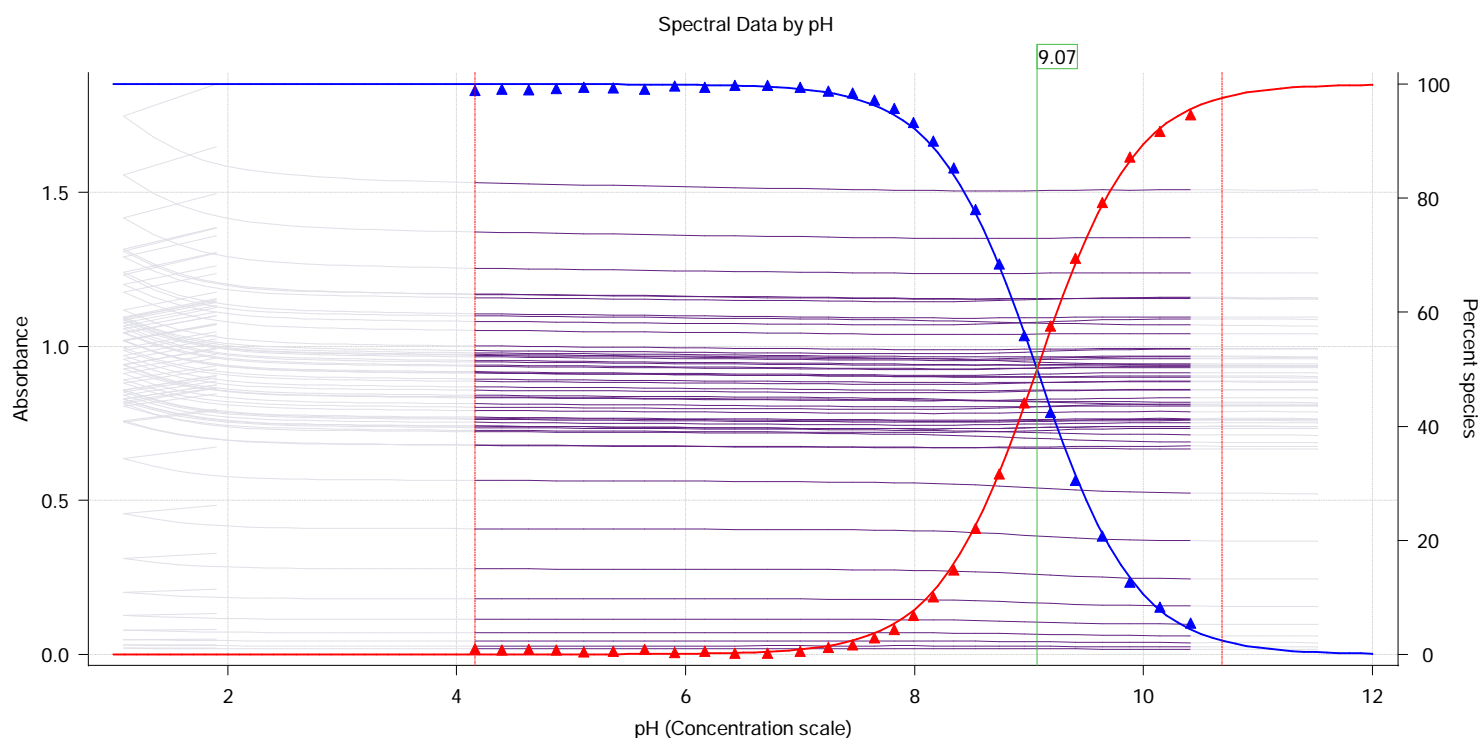
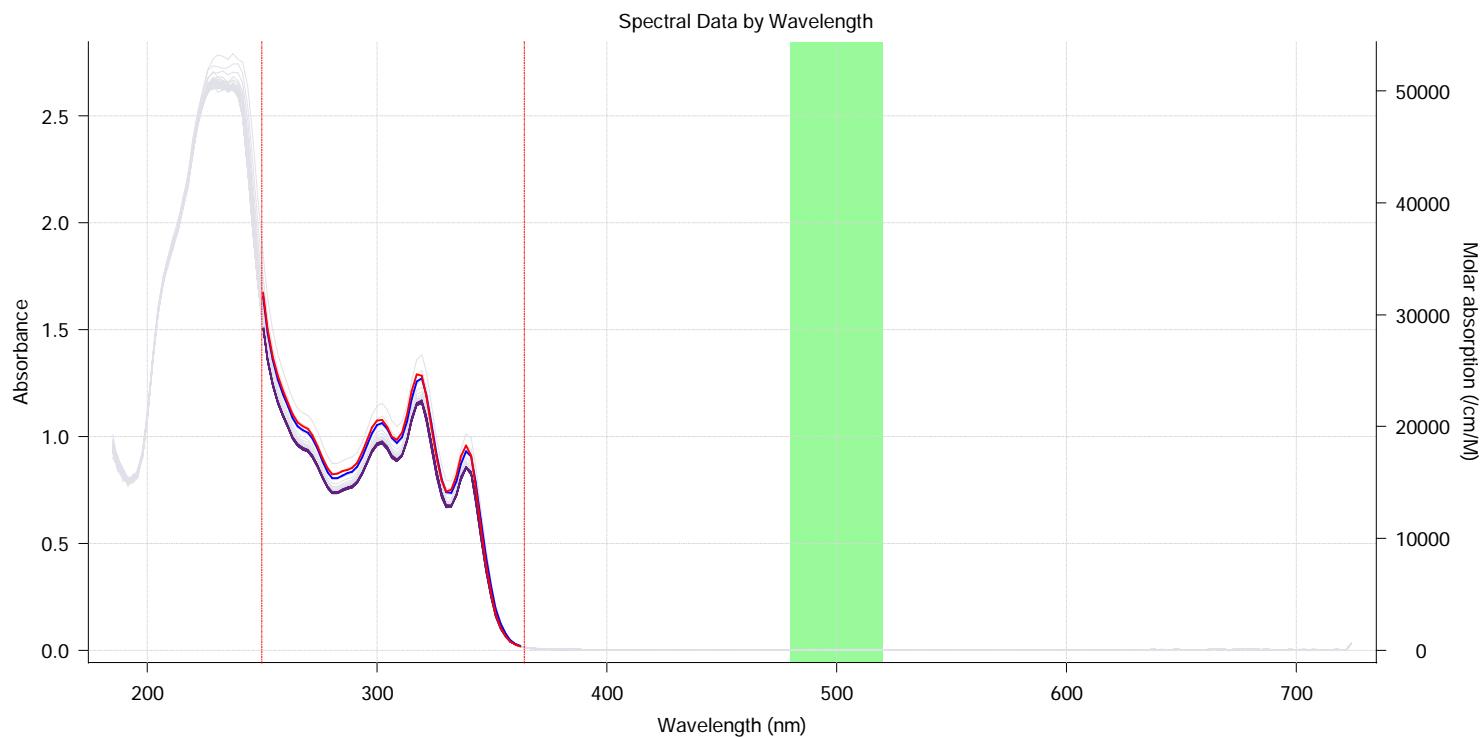


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Fast UV psKa Titration 1 of 3 11H-31014 Points 3 to 53

Graphs

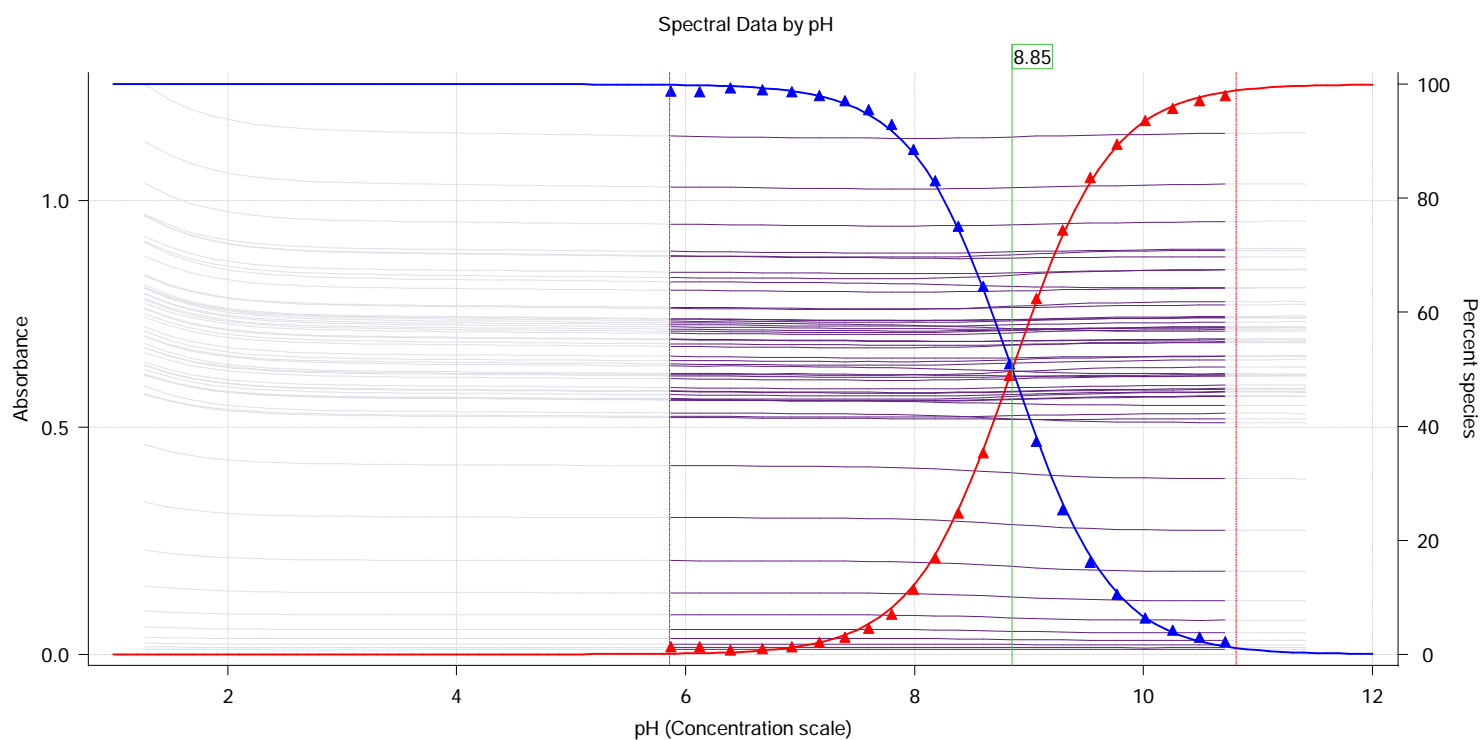
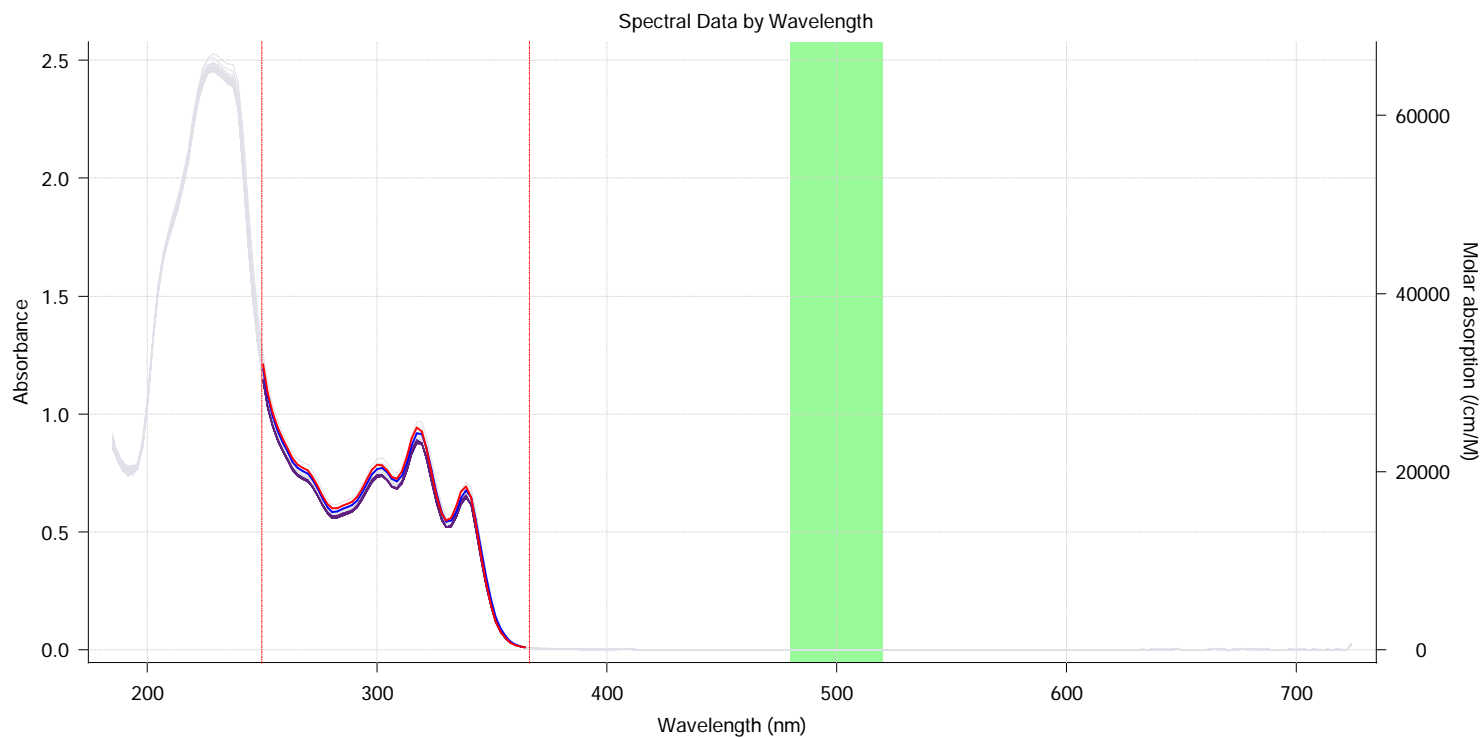


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Fast UV psKa Titration 2 of 3 11H-31014 Points 54 to 104

Graphs

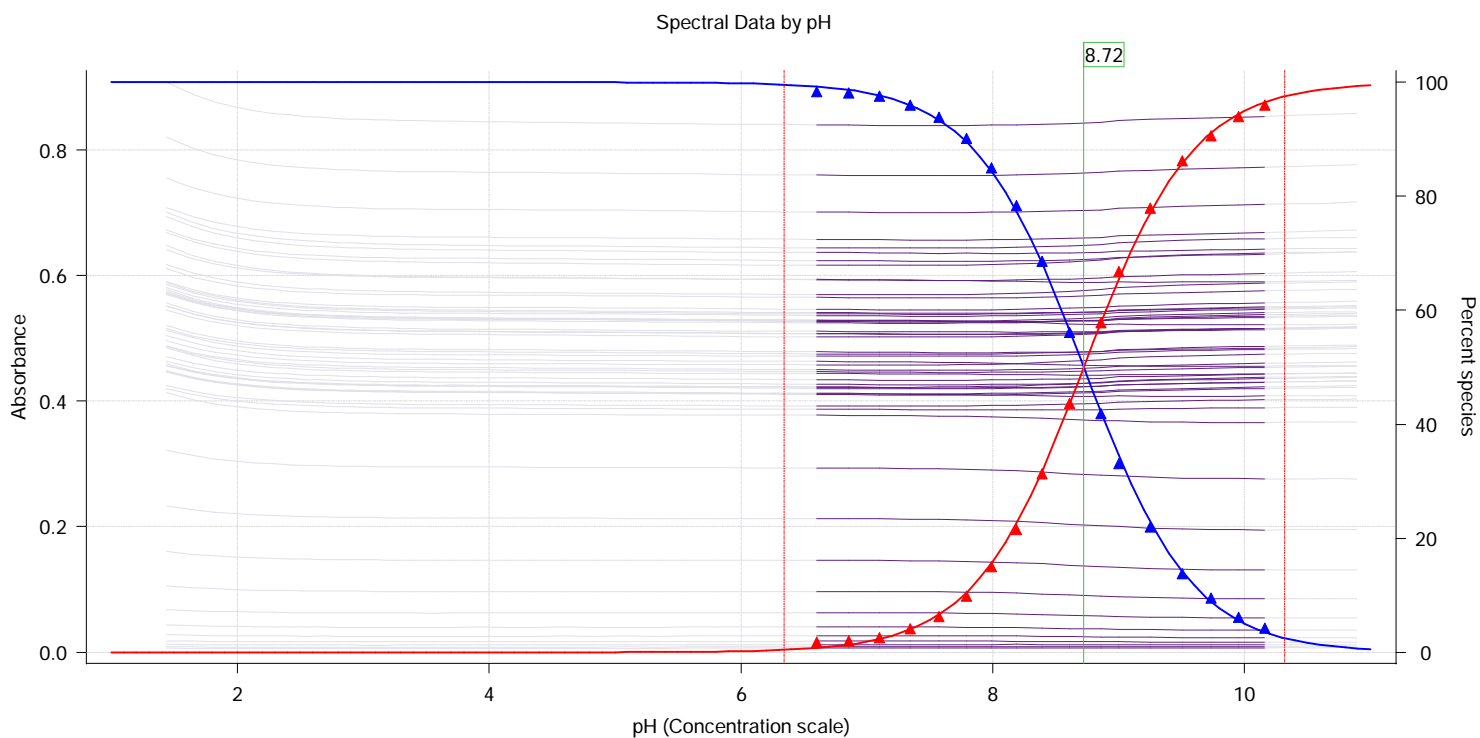
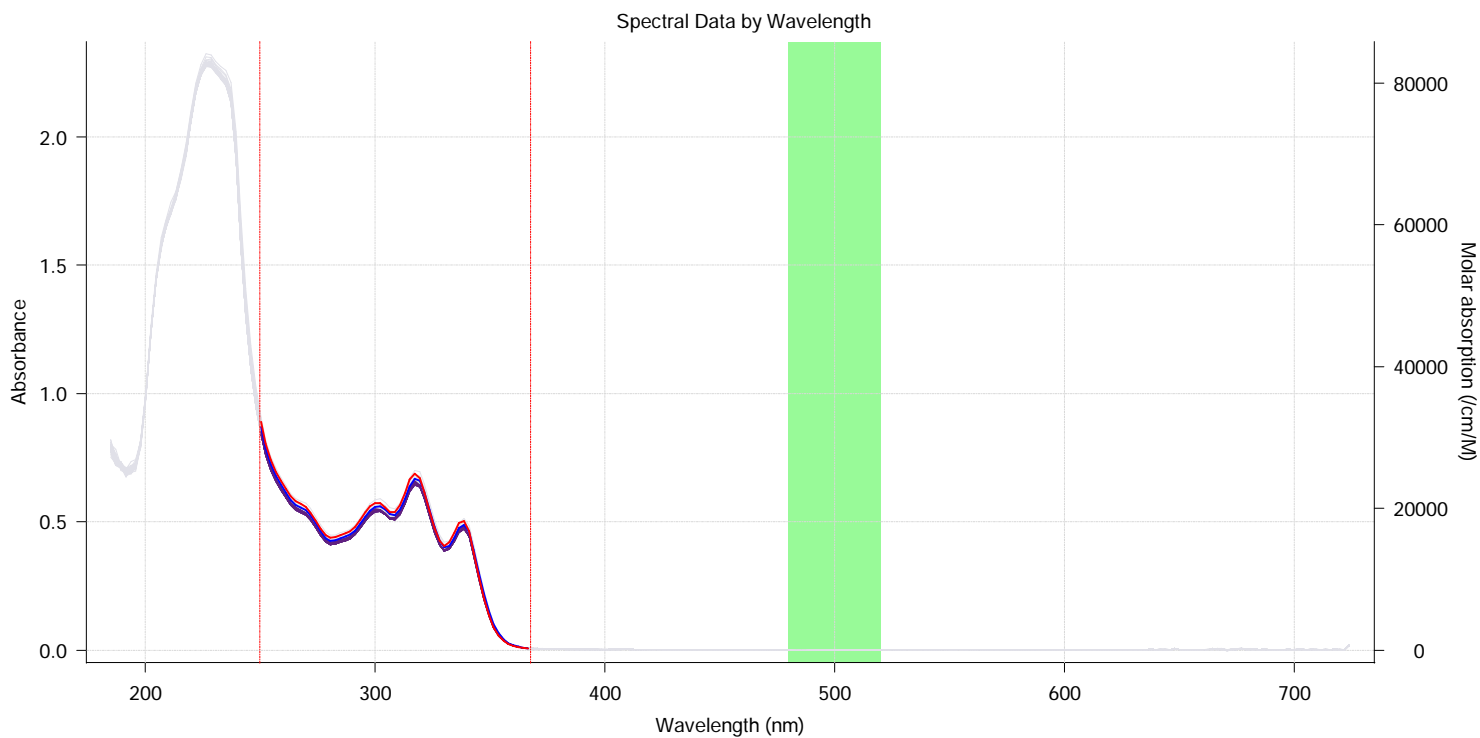


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Fast UV psKa Titration 3 of 3 11H-31014 Points 105 to 154

Graphs





Assay model

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Analyst:
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Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000243		
Sample by	Volume		
Sample volume	0.0100 mL		
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown		
Molecular weight	371.39		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base		
pKa 1	9.00		
logp (XH +)	-10.00		
logP (neutral X)	-10.00		
