



Yasuda-Shedlovsky Result

Sample name: **CS000197**
Assay name: **Fast UV psKa**
Assay ID: **11I-15007**
Filename: **E:\T3 DATA\1109\11I-15007_CS000197_Fast UV psKa.t3r**

Experiment start time: **15/09/2011 10:16:17**
Analyst:
Instrument ID: **T311042**

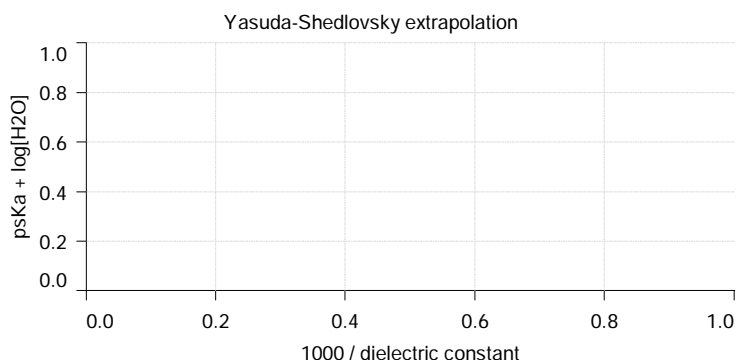
Yasuda-Shedlovsky result

Extrapolation type pKa 0% SD Intercept Slope R² Ionic strength Temperature

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H ₂ O]	Ionic strength	Temperature
11I-15007 Points 107 to 159	19.86 %	Up	UV-metric pKa	76.8	45.1 M	0.206 M	27.1°C
11I-15007 Points 54 to 106	26.74 %	Up	UV-metric pKa	76.7	41.5 M	0.203 M	26.3°C
11I-15007 Points 3 to 53	36.03 %	Up	UV-metric pKa	75.8	36.6 M	0.193 M	26.8°C

Graphs

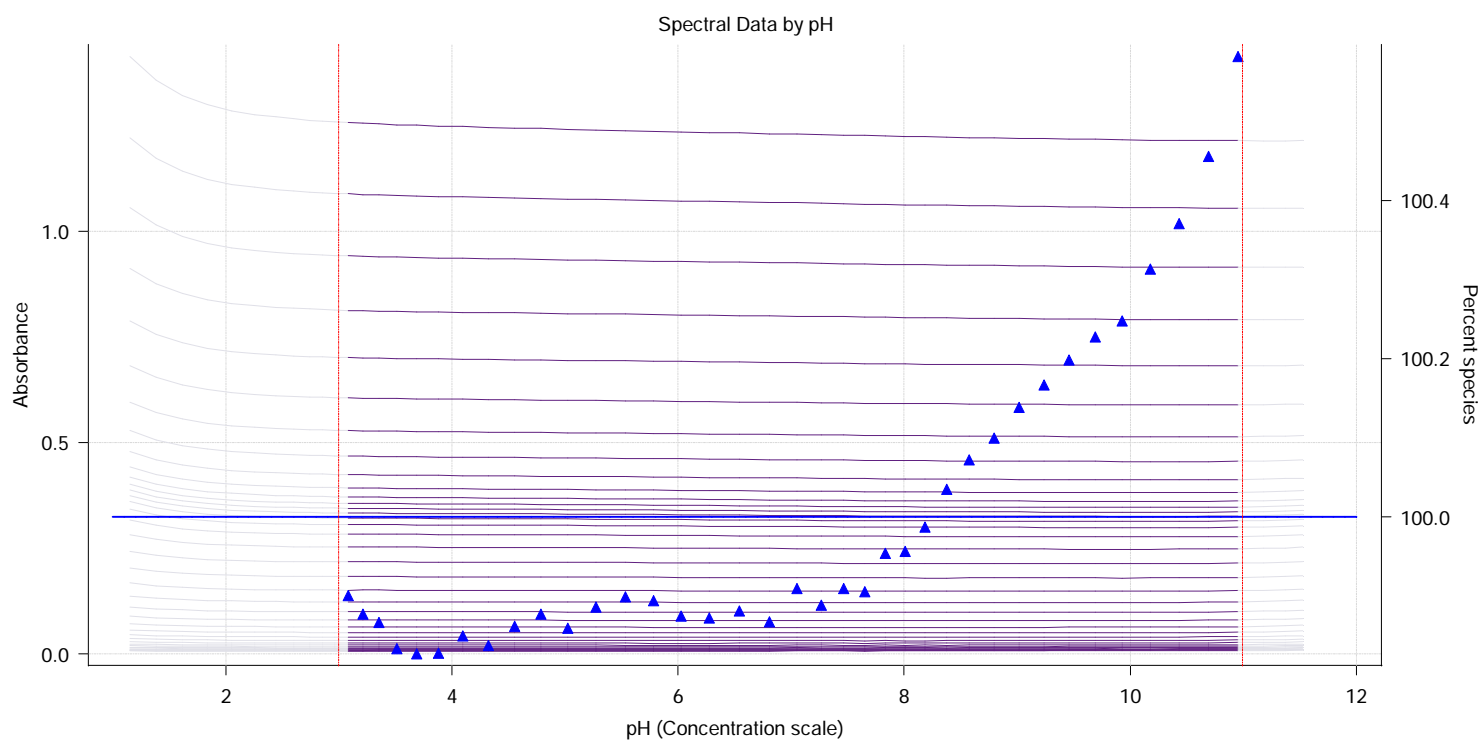
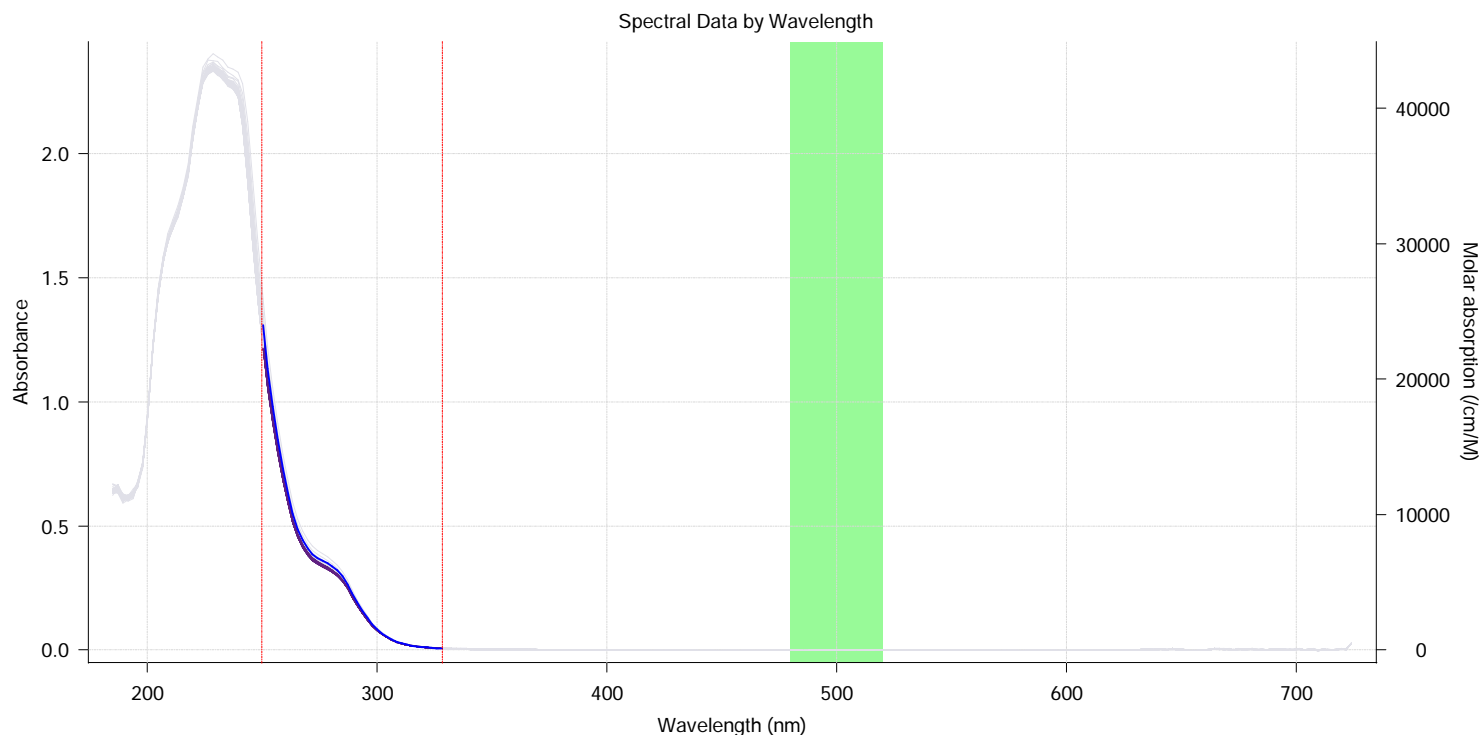


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Fast UV psKa Titration 1 of 3 11I-15007 Points 3 to 53

Graphs

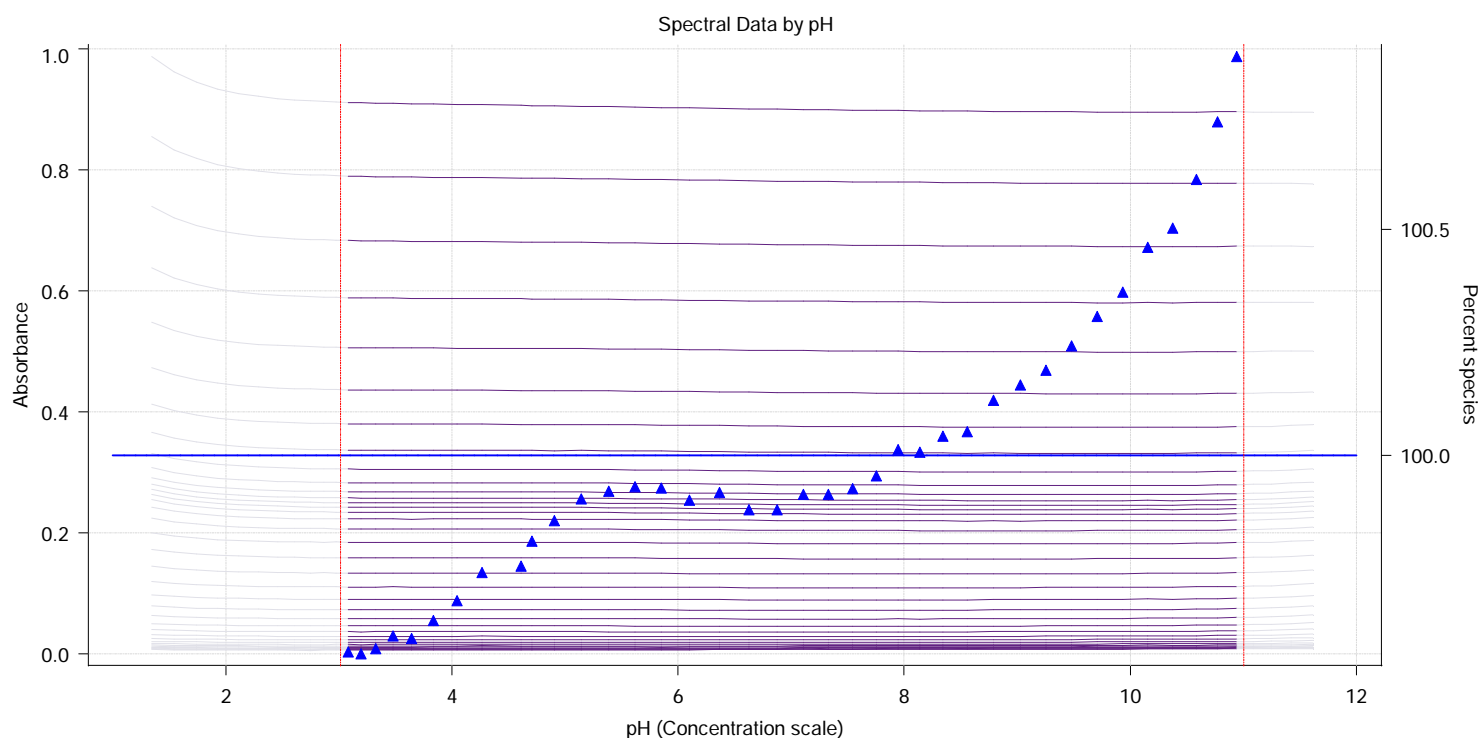
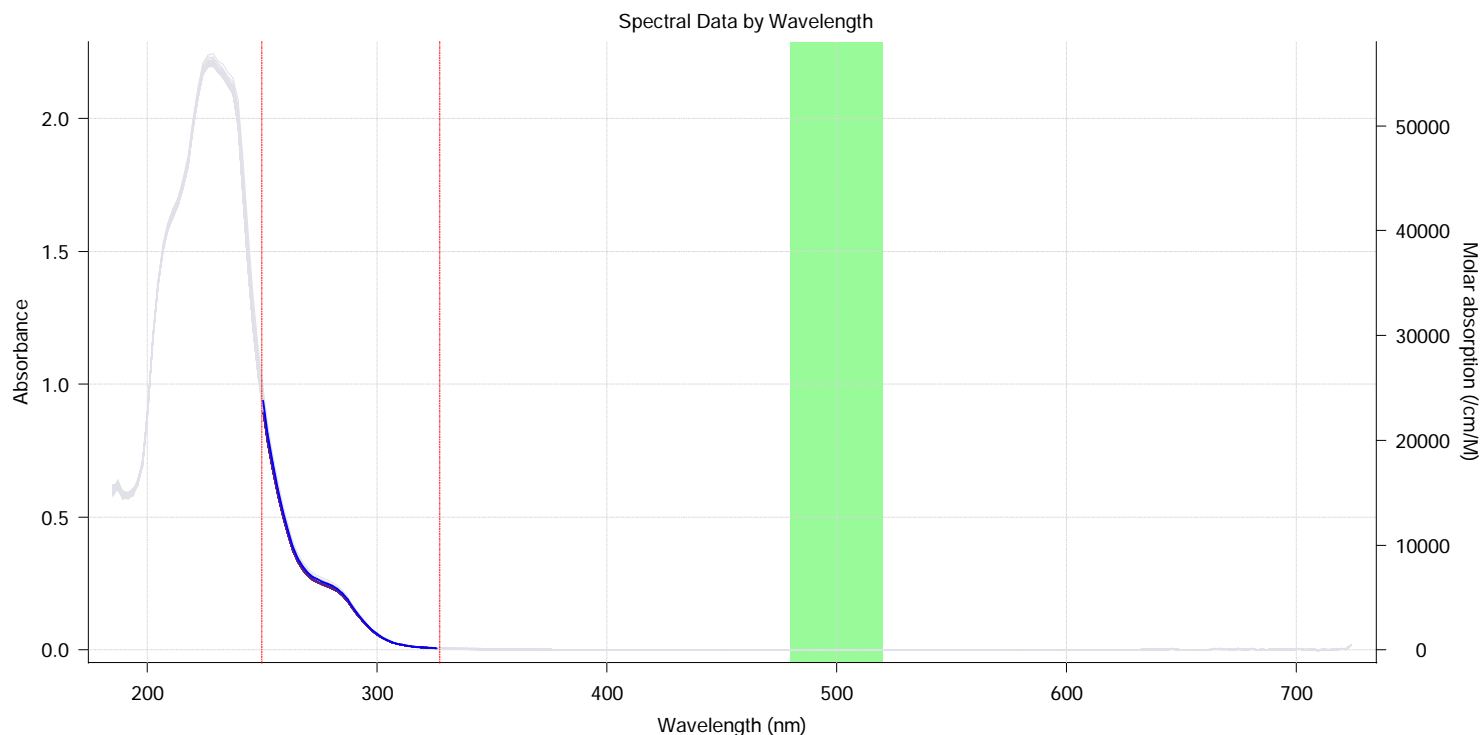


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Fast UV psKa Titration 2 of 3 11I-15007 Points 54 to 106

Graphs

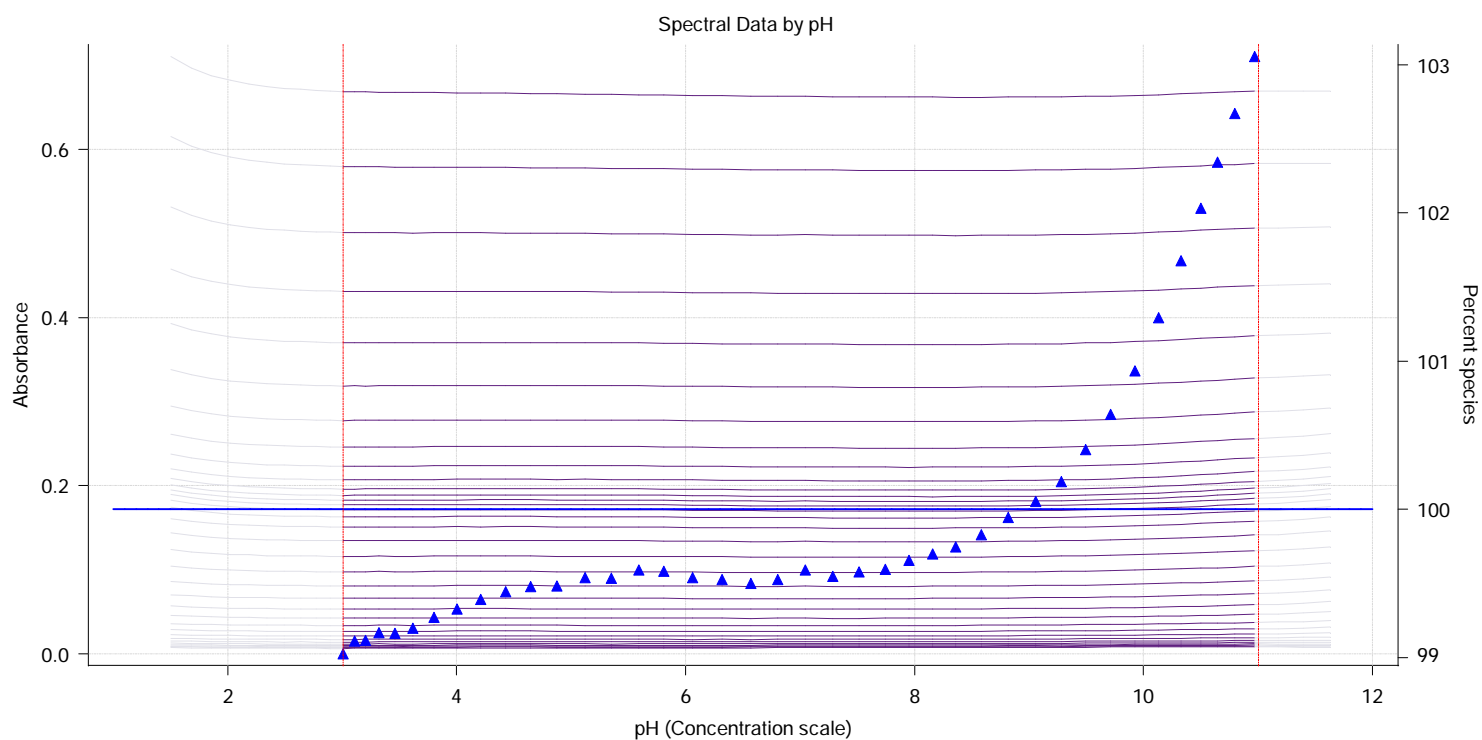
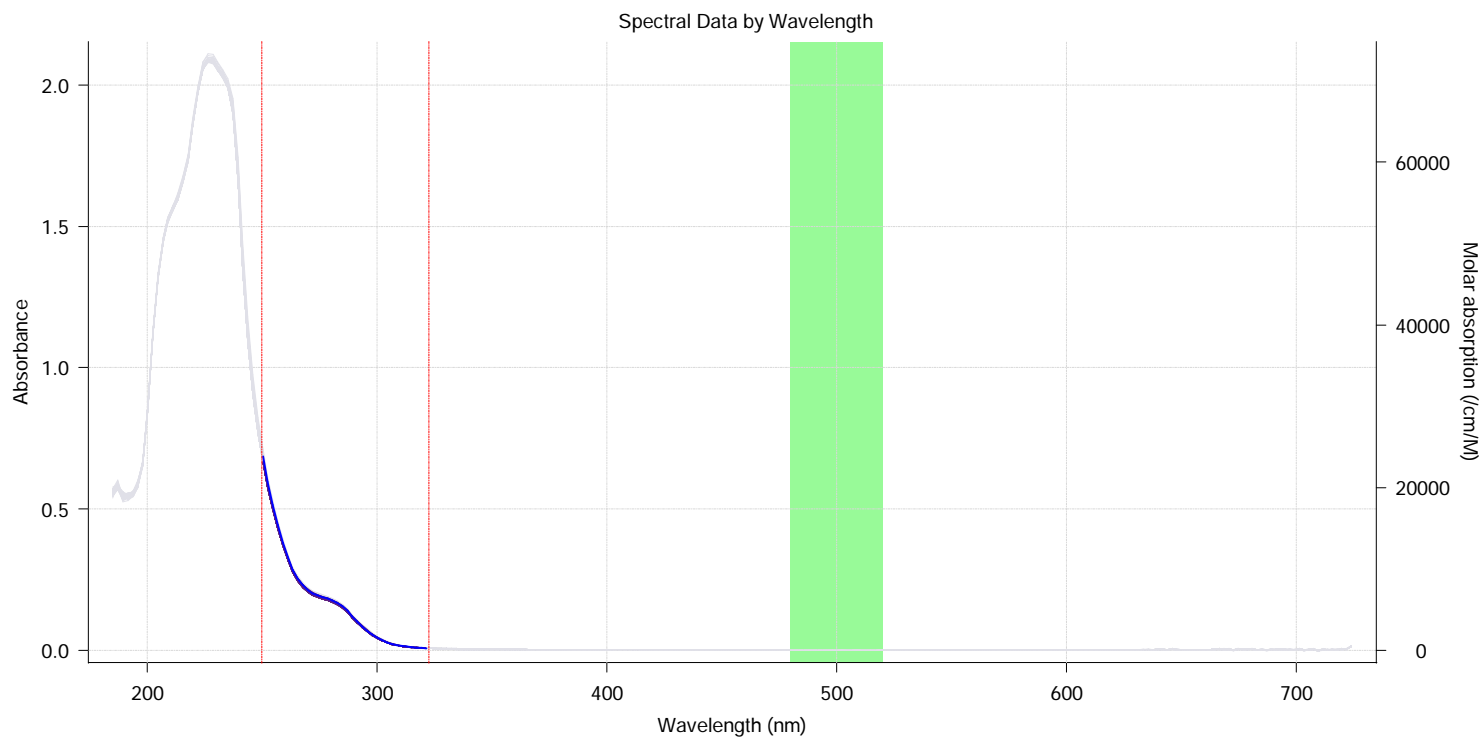


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Fast UV psKa Titration 3 of 3 11I-15007 Points 107 to 159

Graphs





Assay model

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Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000197		
Sample by	Volume	15/09/2011 10:15:02	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
Sample volume	0.0100 mL	15/09/2011 10:15:02	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	15/09/2011 10:15:02	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
Molecular weight	387.49		
Individual pKa ionic environments	No		
Number of pKas	0		
logP (neutral X)	-10.00	15/09/2011 10:15:02	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
