



Yasuda-Shedlovsky Result

Sample name: **CS000275**
Assay name: **Fast UV psKa**
Assay ID: **11H-31021**
Filename: **E:\T3 DATA\1109\20110909-6unstable\CS000275_Fast UV psKa_DMSO-1.t3r**

Experiment start time: **31/08/2011 21:59:16**
Analyst:
Instrument ID: **T311042**

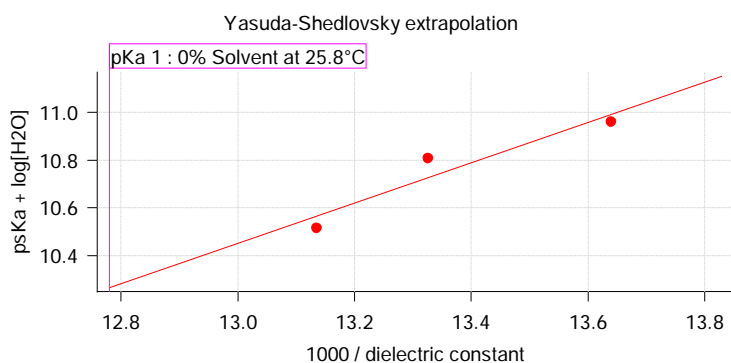
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	8.53	±0.17	-0.44	838.2430	0.9006	0.192 M	25.8°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H ₂ O]	Ionic strength	Temperature	psKa 1
11H-31021 Points 89 to 130	36.81 %	Up	UV-metric pKa	76.1	36.2 M	0.192 M	25.8°C	✓ 8.96
11H-31021 Points 46 to 88	46.90 %	Up	UV-metric pKa	75.0	30.7 M	0.194 M	25.4°C	✓ 9.32
11H-31021 Points 3 to 45	54.88 %	Up	UV-metric pKa	73.3	26.3 M	0.189 M	26.3°C	✓ 9.54

Graphs

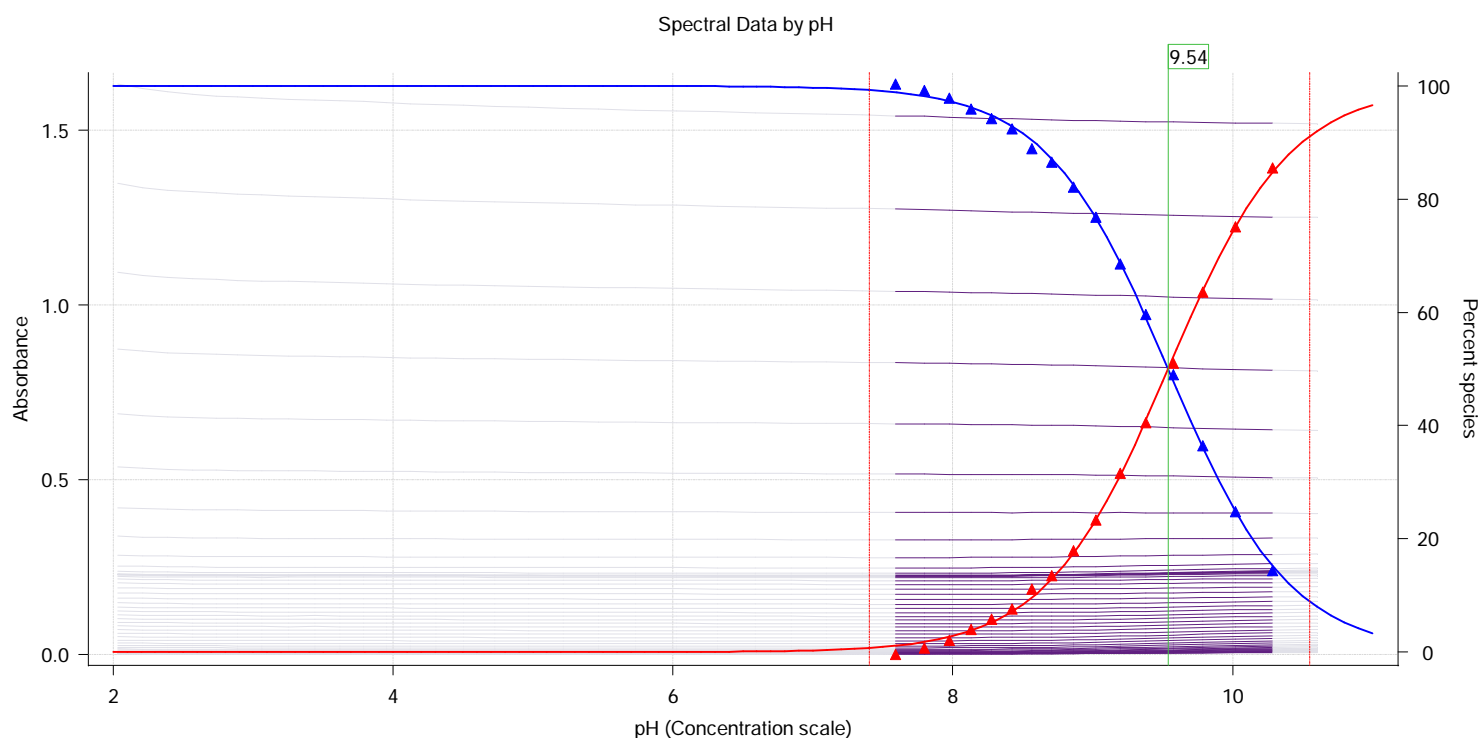
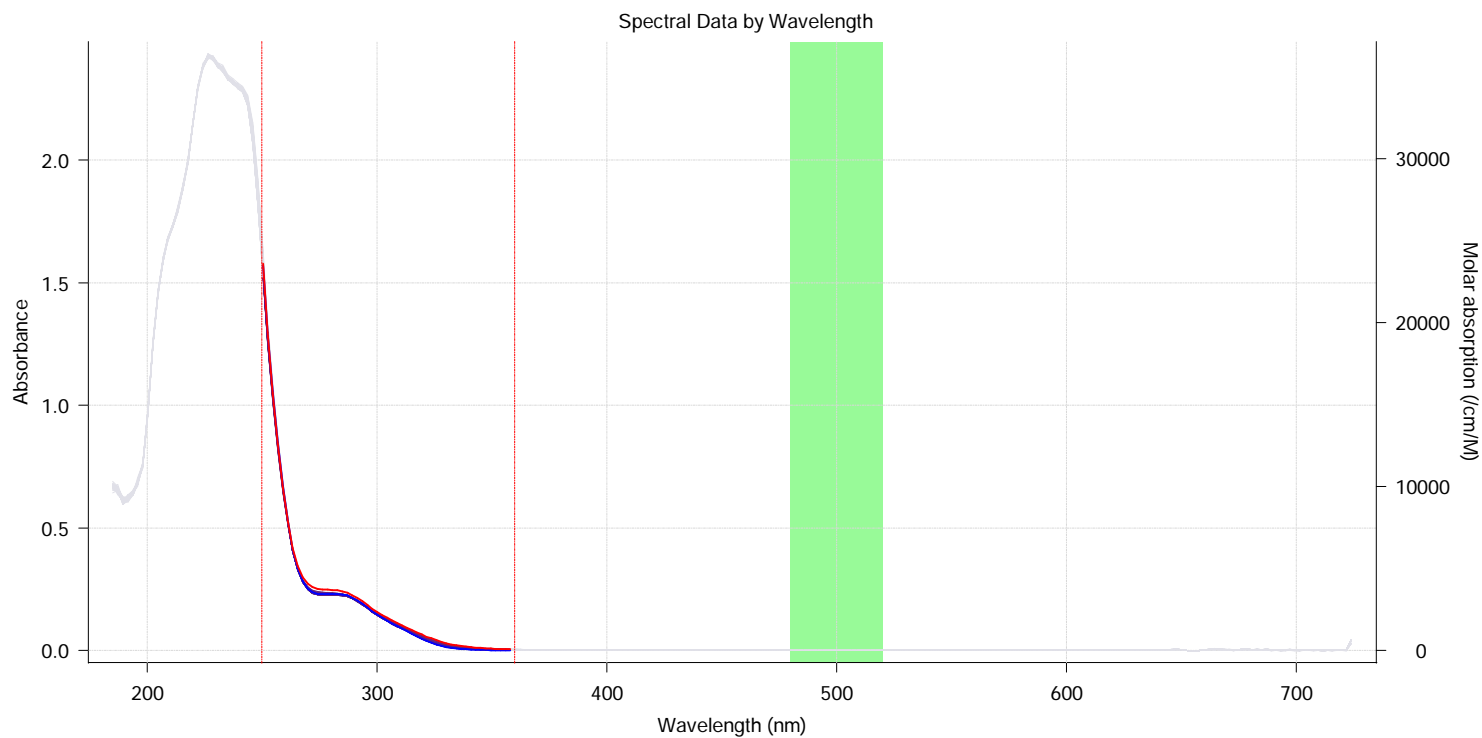


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Fast UV psKa Titration 1 of 3 11H-31021 Points 3 to 45

Graphs

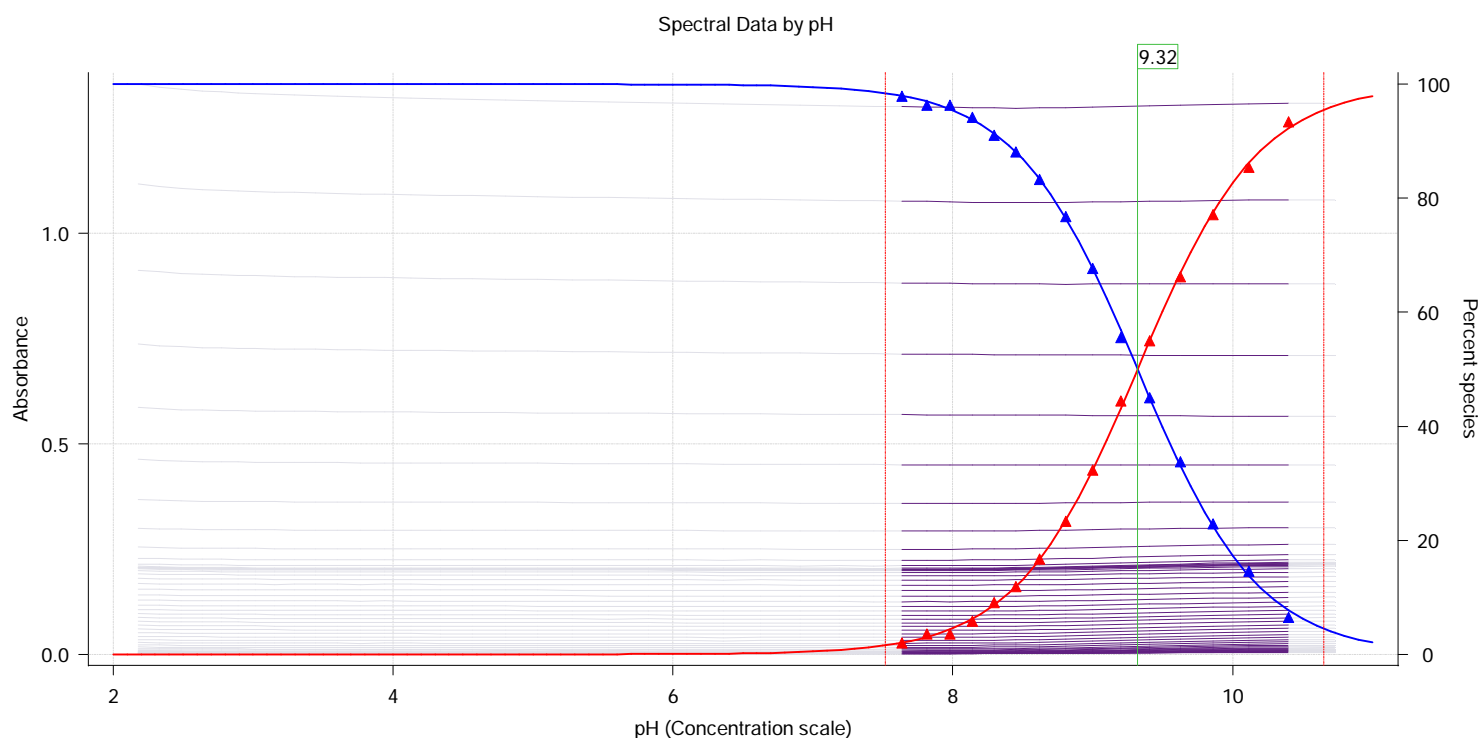
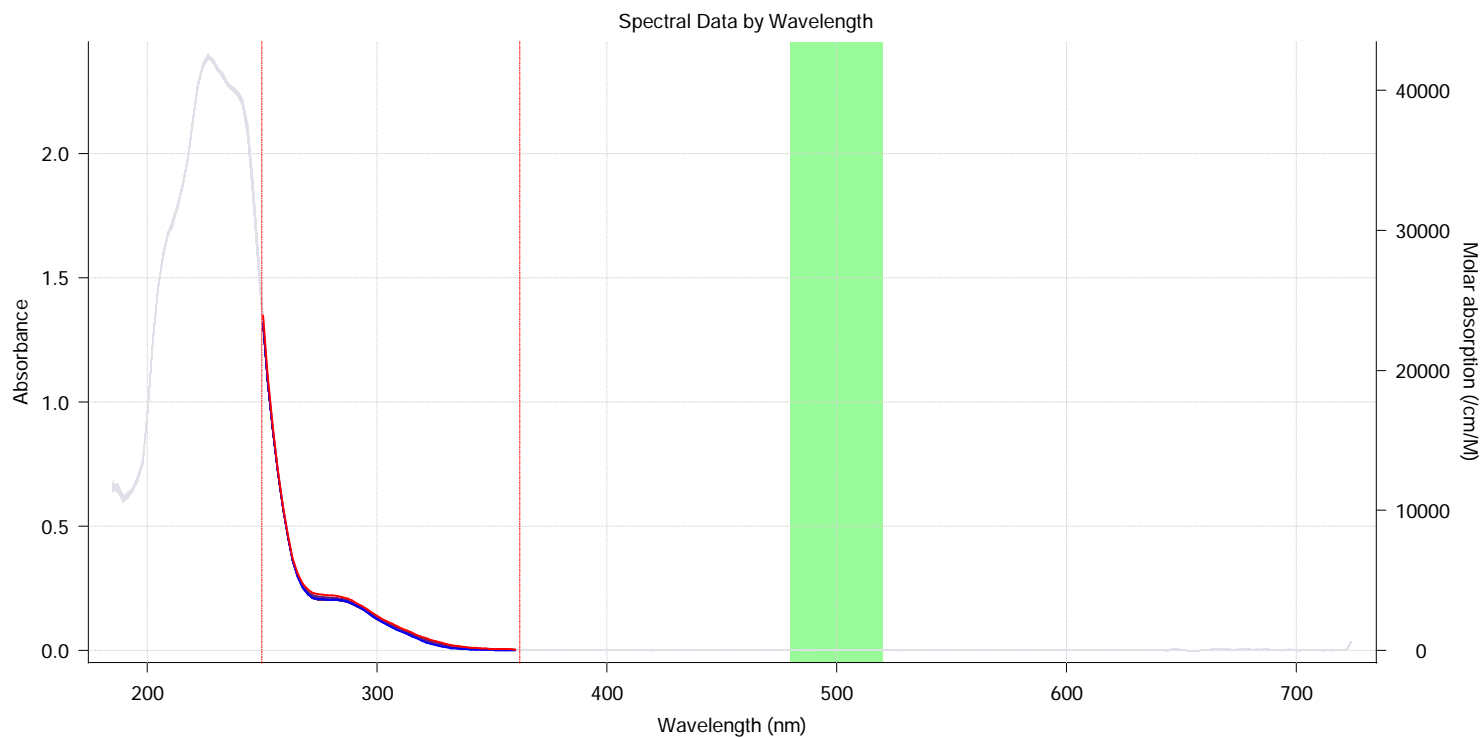


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Fast UV psKa Titration 2 of 3 11H-31021 Points 46 to 88

Graphs

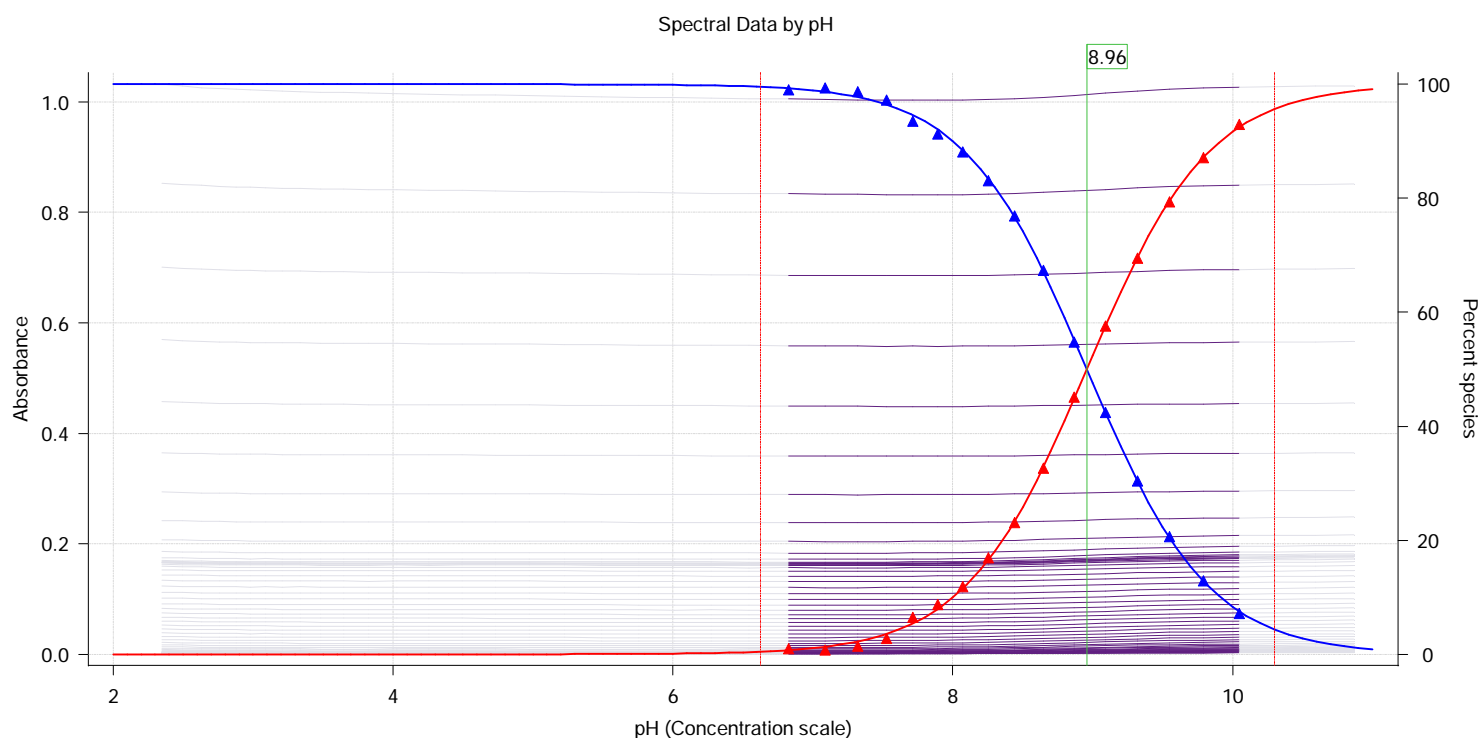
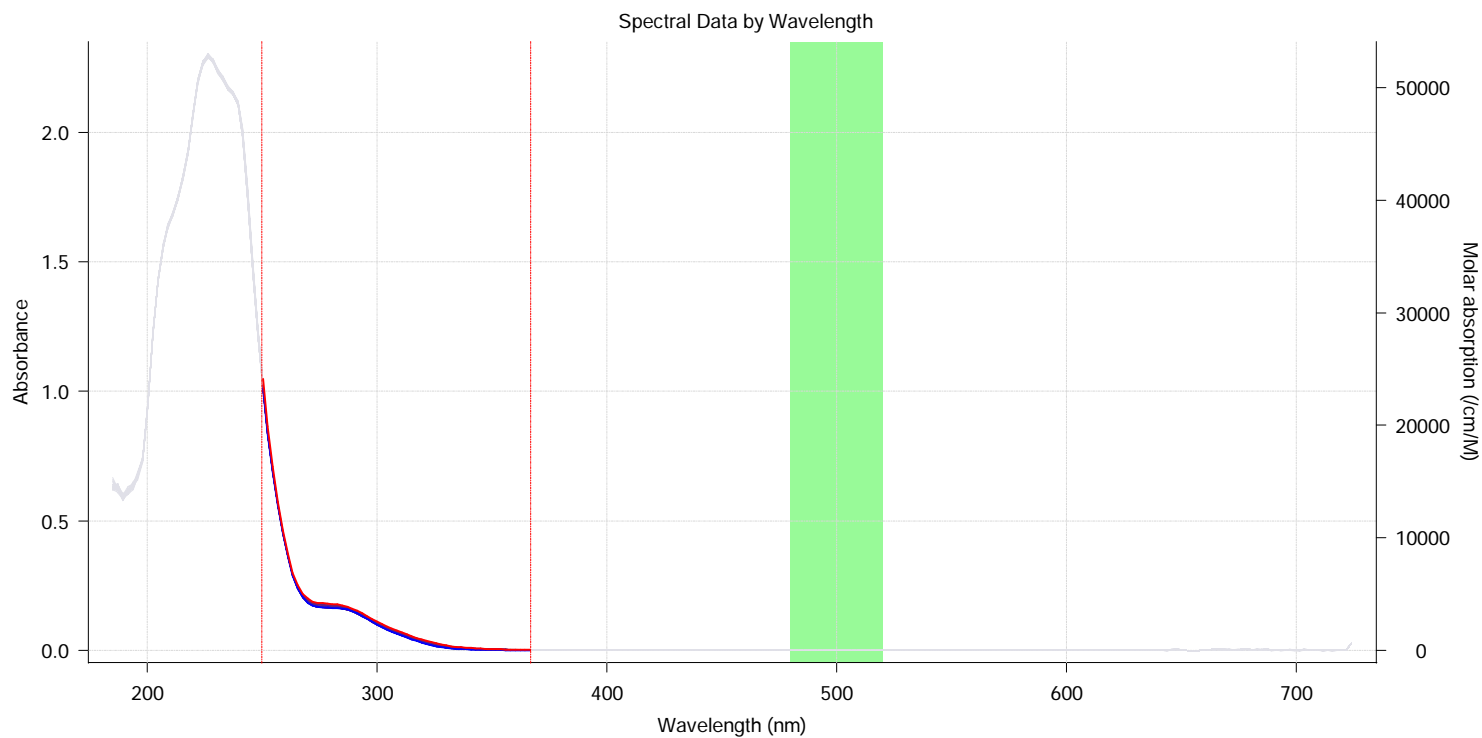


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Fast UV psKa Titration 3 of 3 11H-31021 Points 89 to 130

Graphs





Assay model

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Instrument ID: **T311042**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000275		
Sample by	Volume	31/08/2011 20:48:17	E:\T3 DATA\1108\11H-31014_CS000243_Fast UV psKa.t3r
Sample volume	0.0100 mL	31/08/2011 20:48:17	E:\T3 DATA\1108\11H-31014_CS000243_Fast UV psKa.t3r
Solvent	DMSO		
Sample concentration	0.010000 M		
Solubility	Unknown	31/08/2011 20:48:17	E:\T3 DATA\1108\11H-31014_CS000243_Fast UV psKa.t3r
Molecular weight	340.71		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	31/08/2011 20:48:17	E:\T3 DATA\1108\11H-31014_CS000243_Fast UV psKa.t3r
pKa 1	8.60		
logp (XH +)	-10.00	31/08/2011 20:48:17	E:\T3 DATA\1108\11H-31014_CS000243_Fast UV psKa.t3r
logP (neutral X)	-10.00		
