

Sample name: **CS000252**
 Assay name: **Fast UV psKa**
 Assay ID: **11I-15018**
 Filename: **E:\T3 DATA\1109\11I-15018_CS000252_Fast UV psKa.t3r**

Experiment start time: **15/09/2011 16:30:08**
 Analyst:
 Instrument ID: **T311042**

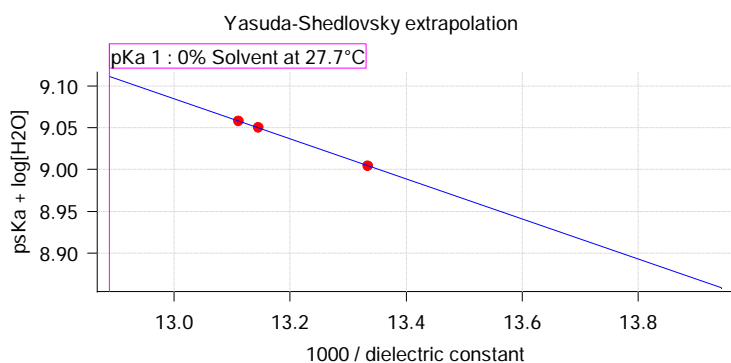
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	7.37	±0.00	12.19	-238.9021	1.0000	0.210 M	27.7°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H ₂ O]	Ionic strength	Temperature	psKa 1
11I-15018 Points 129 to 192	22.72 %	Up	UV-metric pKa	76.3	43.6 M	0.214 M	28.2°C	7.42
11I-15018 Points 65 to 128	30.71 %	Up	UV-metric pKa	76.1	39.4 M	0.212 M	27.4°C	7.45
11I-15018 Points 3 to 64	42.13 %	Up	UV-metric pKa	75.0	33.3 M	0.204 M	27.4°C	7.48

Graphs

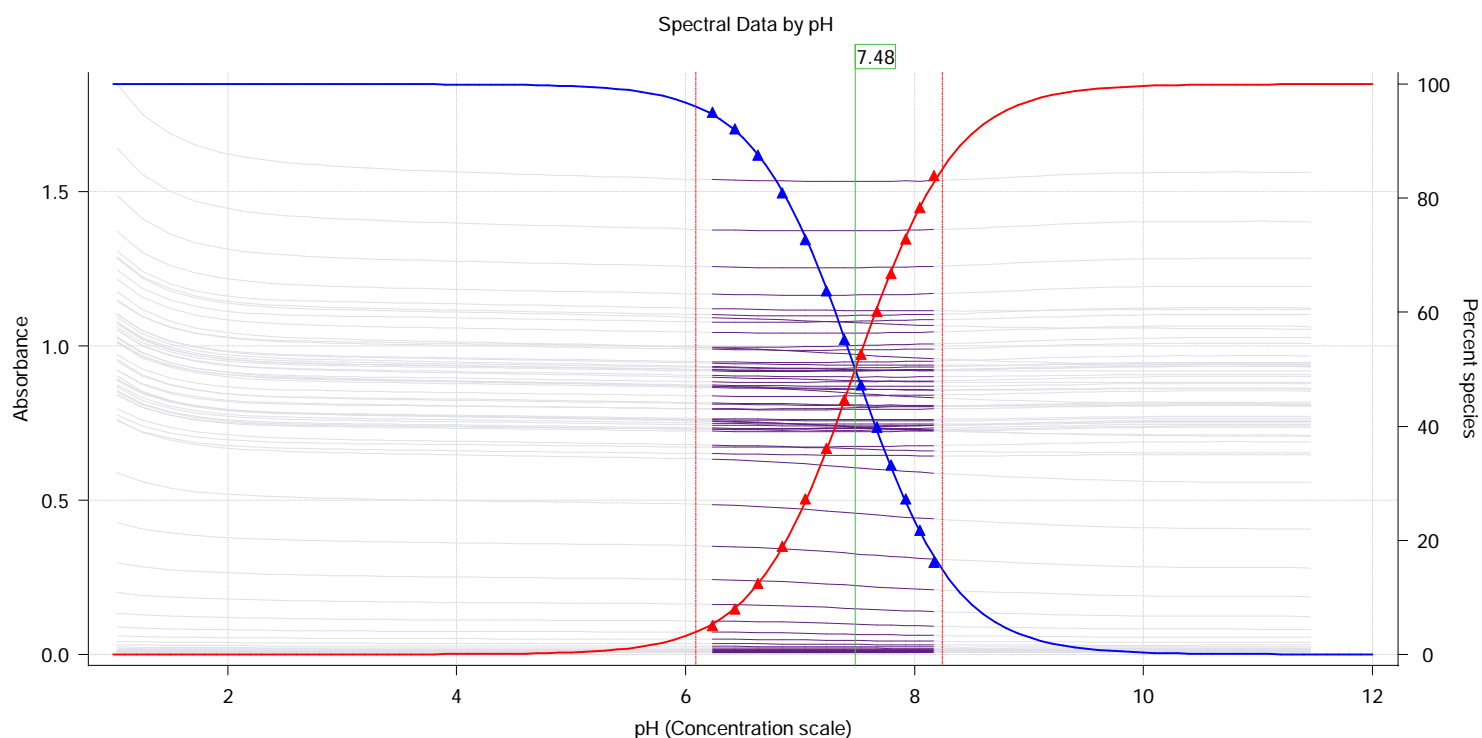
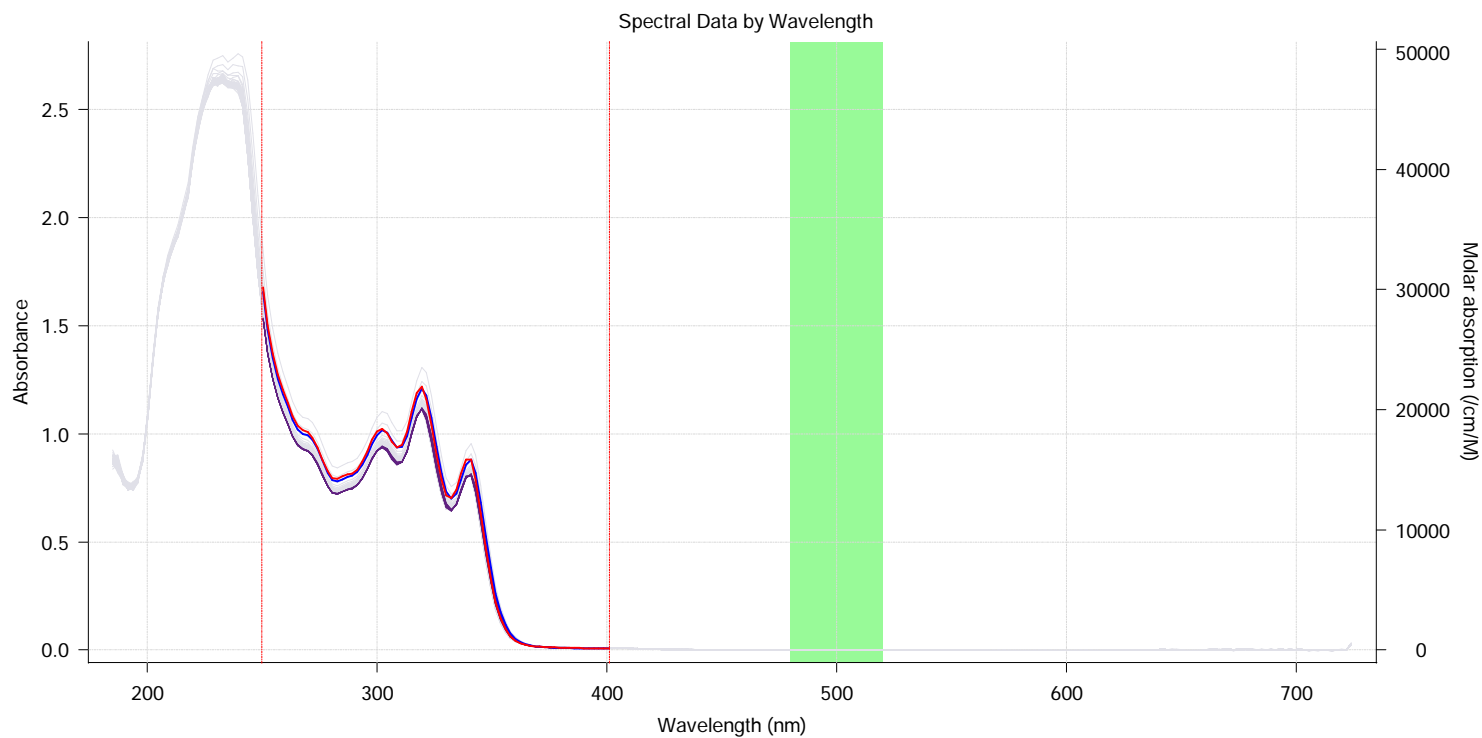


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Fast UV psKa Titration 1 of 3 11I-15018 Points 3 to 64

Graphs

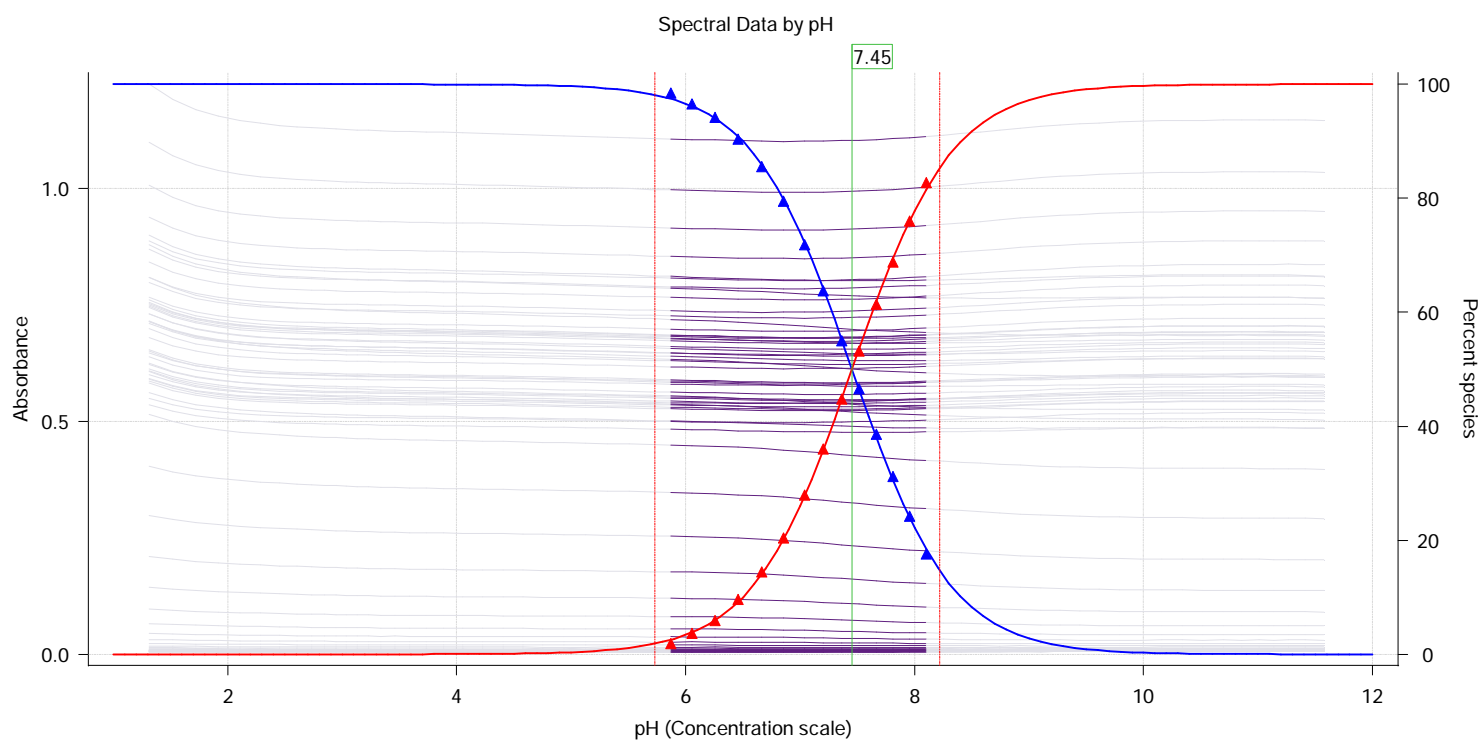
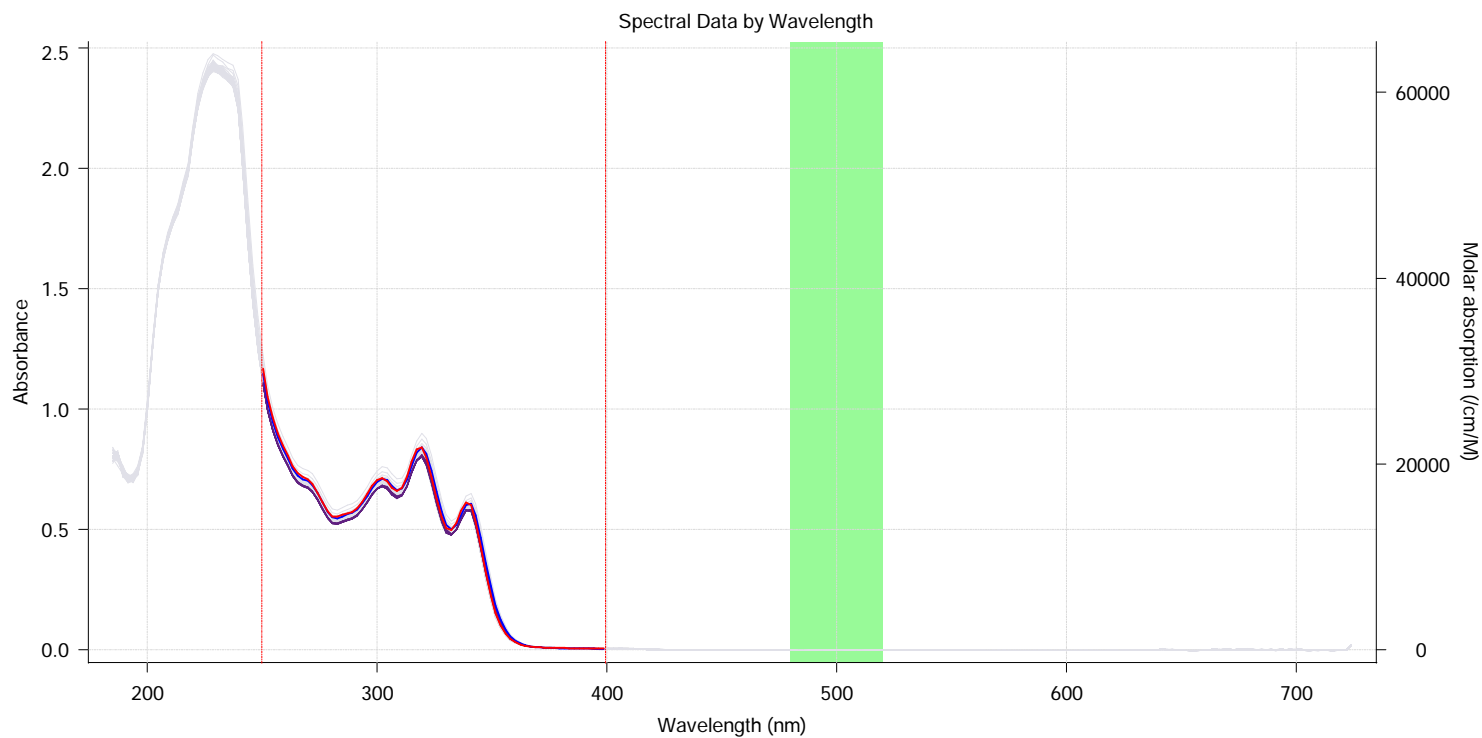


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Fast UV psKa Titration 2 of 3 11I-15018 Points 65 to 128

Graphs

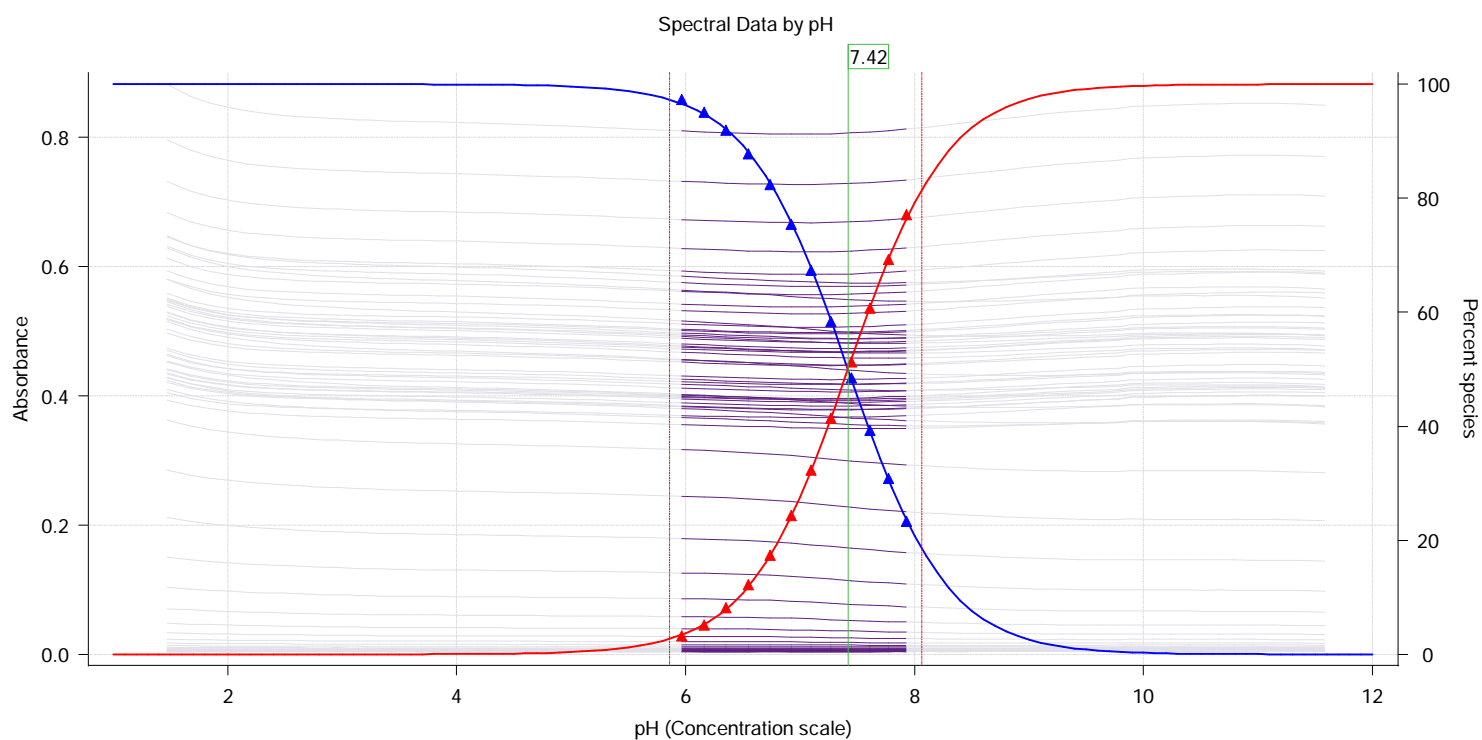
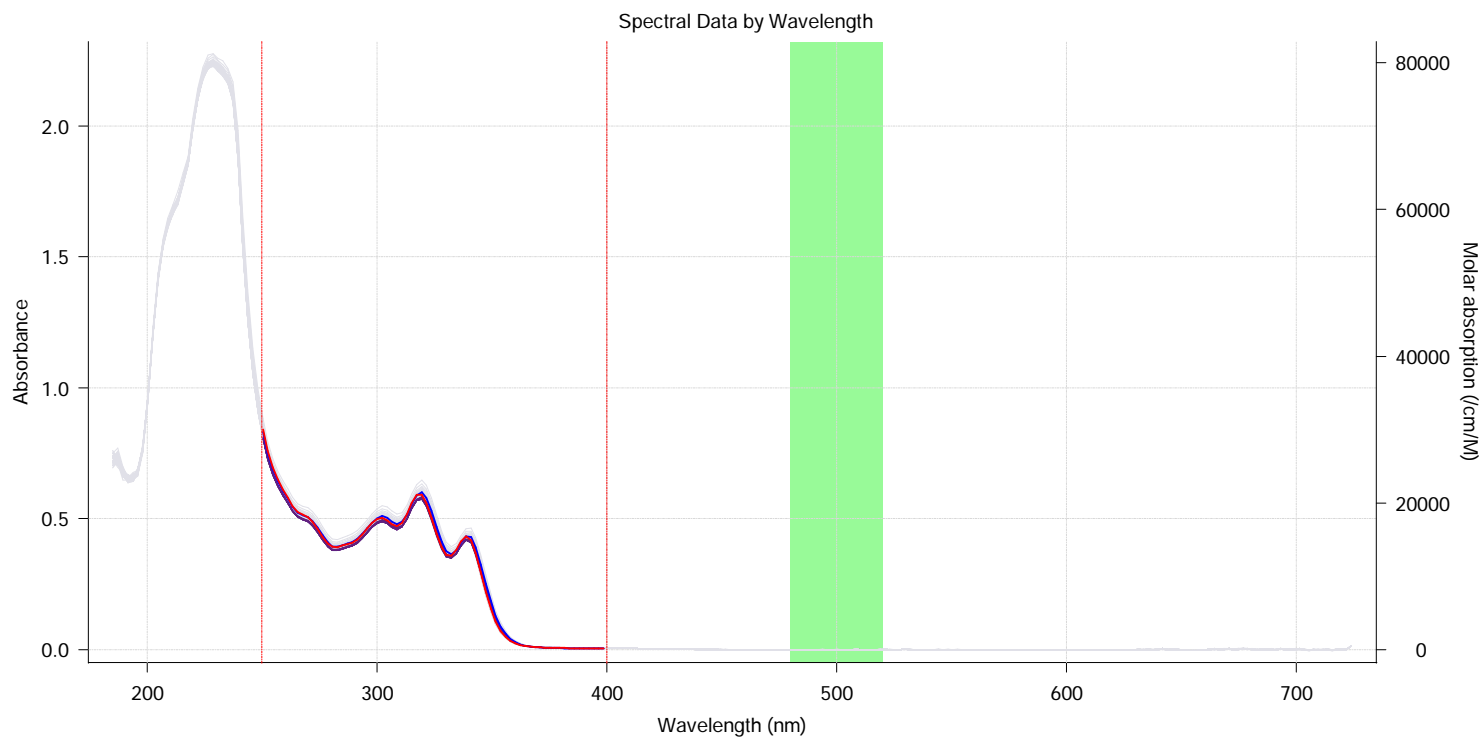


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Fast UV psKa Titration 3 of 3 11I-15018 Points 129 to 192

Graphs





Assay model

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Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000252		
Sample by	Volume		
Sample volume	0.0100 mL		
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	347.37		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	15/09/2011 10:15:02	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
pKa 1	9.65		
logp (XH +)	-10.00	15/09/2011 10:15:02	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
logP (neutral X)	-10.00	15/09/2011 10:15:02	E:\T3 DATA\1109\11I-01002_CS000275_Clean up.t3r
