



## Yasuda-Shedlovsky Result

Sample name: **CS000270**  
Assay name: **Fast UV psKa**  
Assay ID: **11I-15019**  
Filename: **E:\T3 DATA\1109\11I-15019\_CS000270\_Fast UV psKa.t3r**

Experiment start time: **15/09/2011 16:58:33**  
Analyst:  
Instrument ID: **T311042**

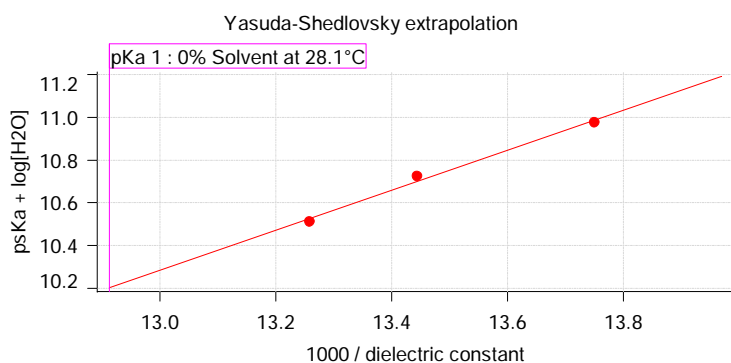
### Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R <sup>2</sup>	Ionic strength	Temperature
Yasuda-Shedlovsky	8.46	±0.05	-1.86	934.2415	0.9911	0.190 M	28.1°C

### Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H <sub>2</sub> O]	Ionic strength	Temperature	psKa 1
11I-15019 Points 89 to 130	36.10 %	Up	UV-metric pKa	75.4	36.5 M	0.190 M	28.0°C	✓ 8.95
11I-15019 Points 46 to 88	45.32 %	Up	UV-metric pKa	74.4	31.5 M	0.192 M	28.0°C	✓ 9.23
11I-15019 Points 3 to 45	54.75 %	Up	UV-metric pKa	72.7	26.3 M	0.188 M	28.2°C	✓ 9.56

### Graphs

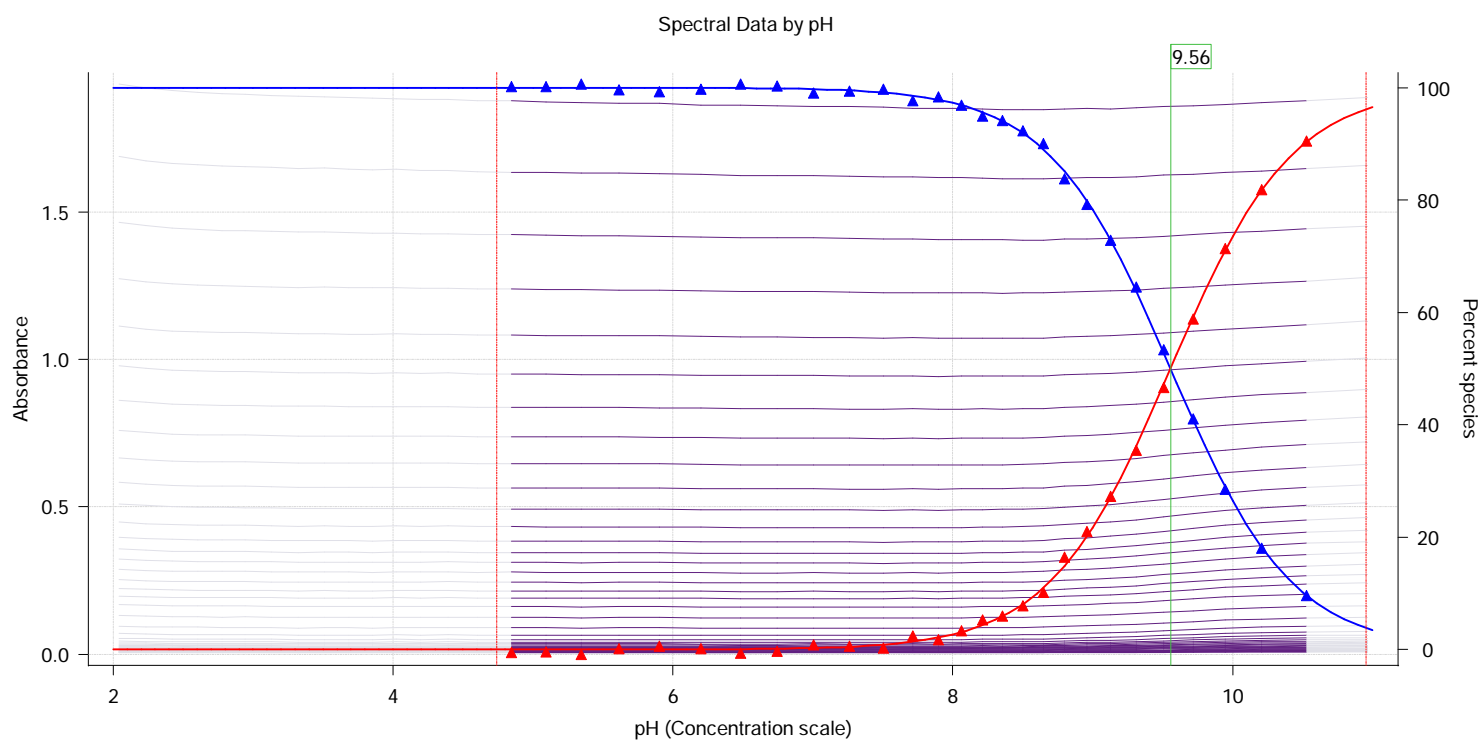
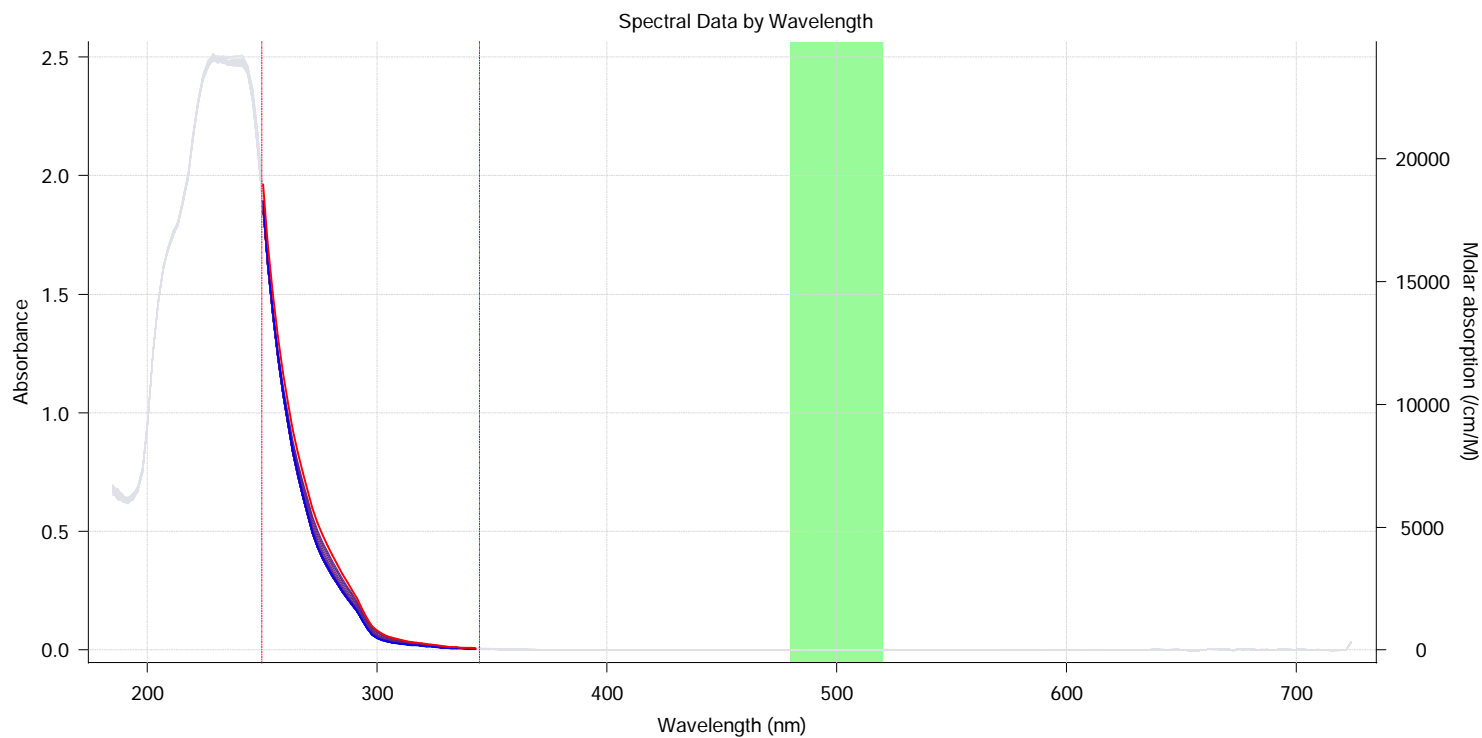


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## Fast UV psKa Titration 1 of 3 11I-15019 Points 3 to 45

### Graphs

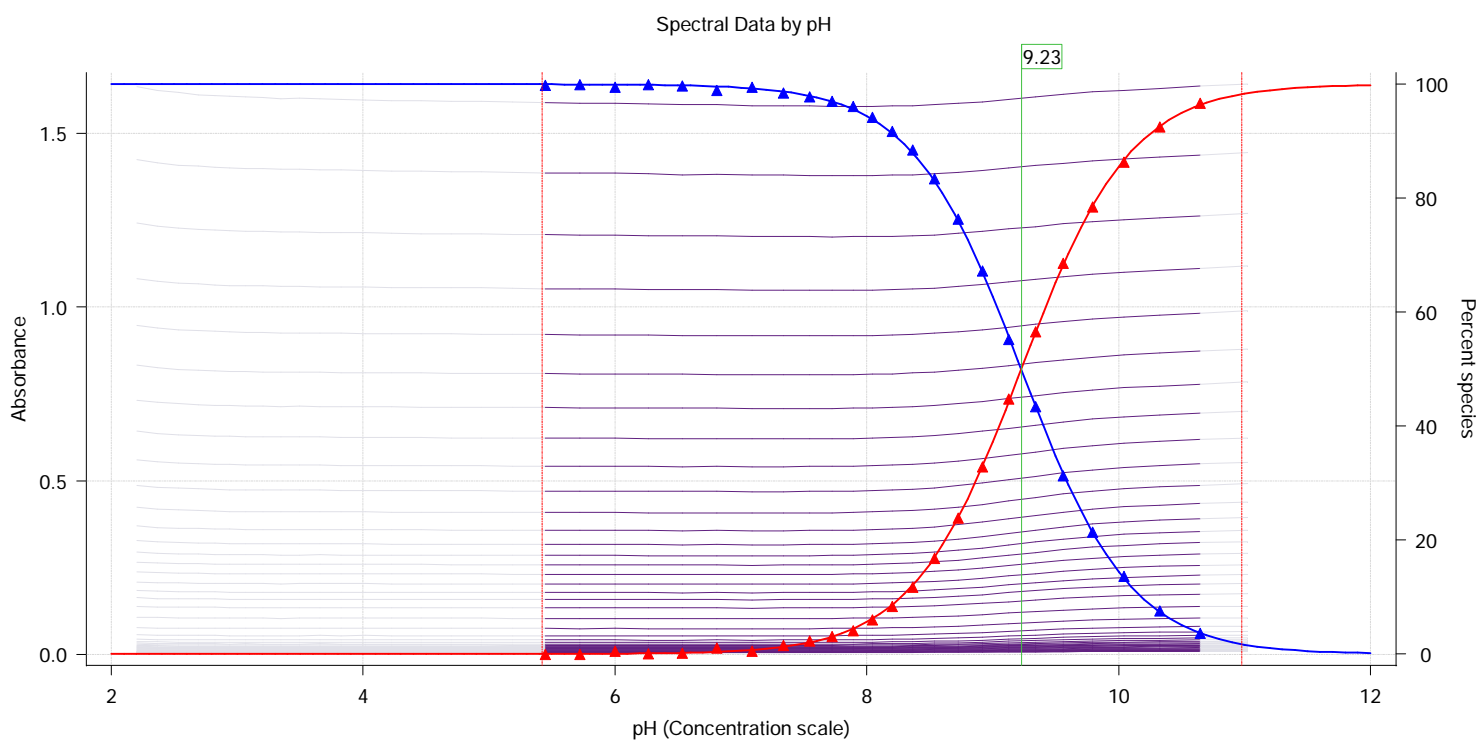
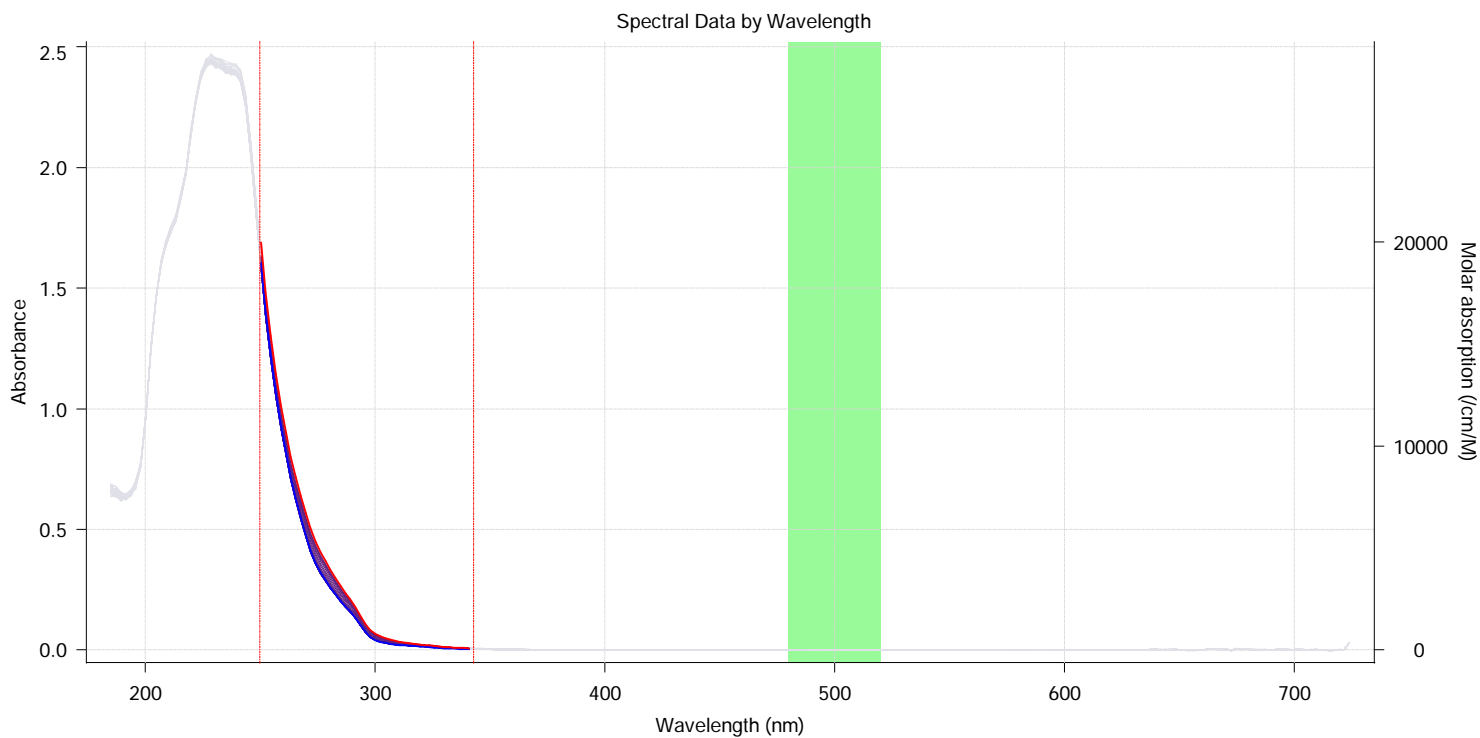


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## Fast UV psKa Titration 2 of 3 11I-15019 Points 46 to 88

### Graphs

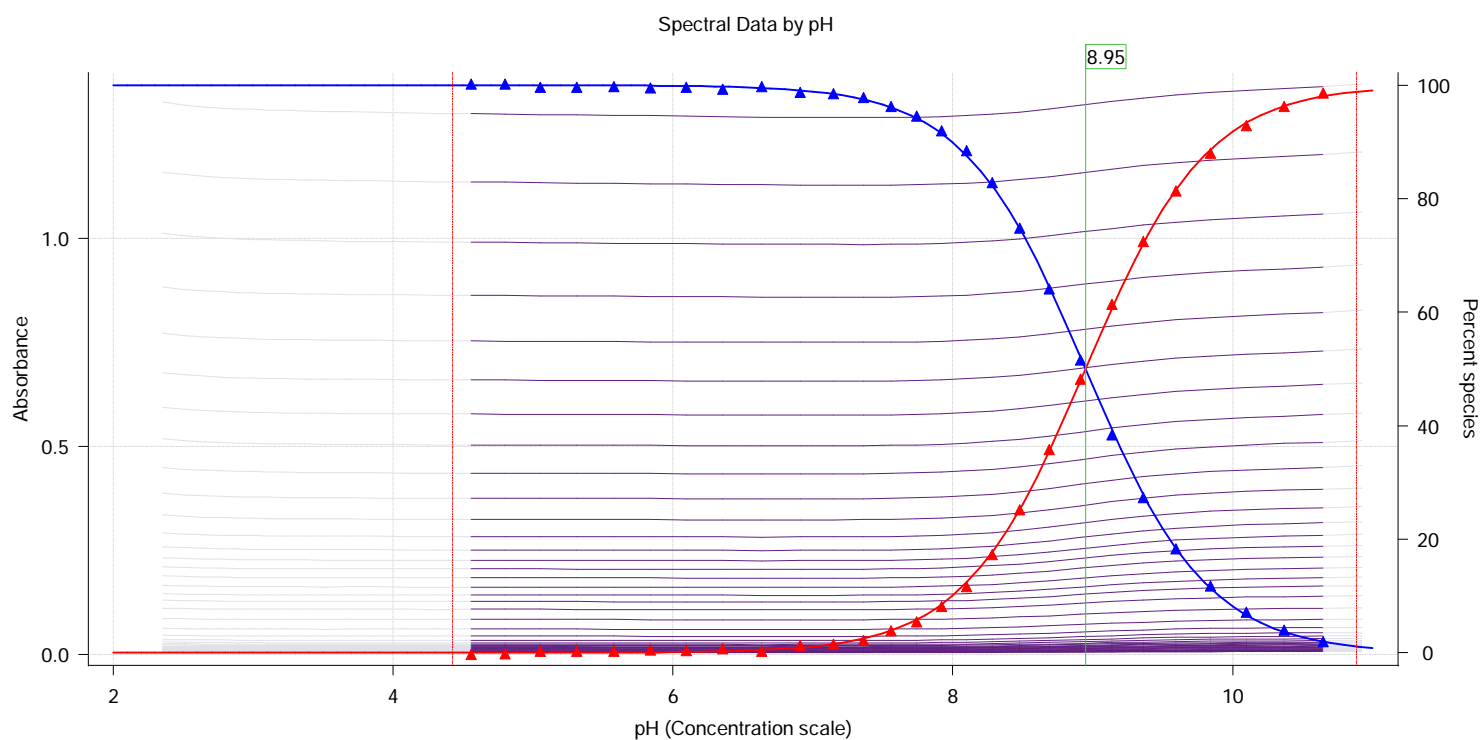
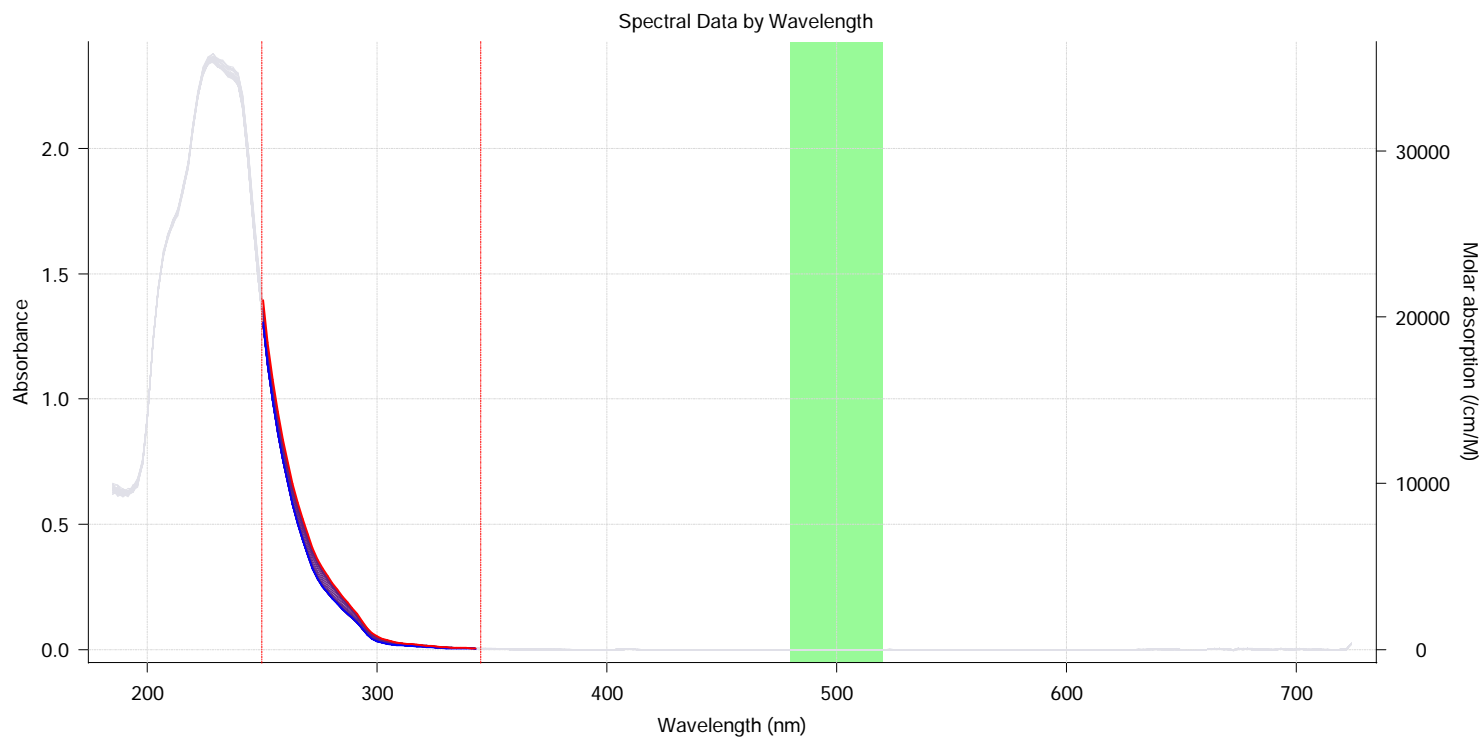


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## Fast UV psKa Titration 3 of 3 11I-15019 Points 89 to 130

### Graphs





## Assay model

Sample name: **CS000270**  
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### Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000270		
Sample by	Volume		
Sample volume	0.0150 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	324.64		
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

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