



Yasuda-Shedlovsky Result

Sample name: **CS000197**
Assay name: **pH-metric psKa**
Assay ID: **11I-13010**
Filename: **E:\T3 DATA\1109\11I-13010_CS000197_pH-metric psKa.t3r**

Experiment start time: **13/09/2011 16:31:36**
Analyst:
Instrument ID: **T311042**

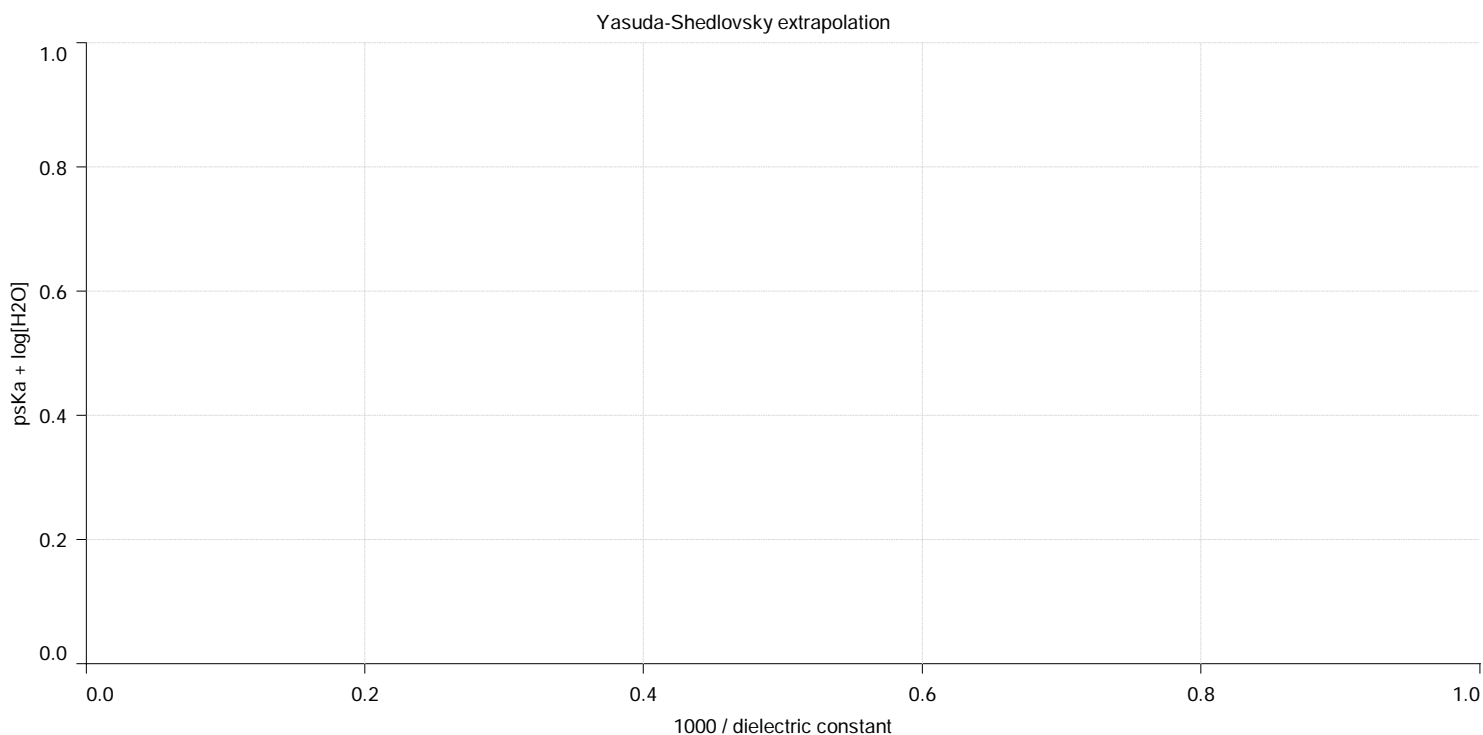
Yasuda-Shedlovsky result

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

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H ₂ O]	Ionic strength	Temperature
11I-13010 Points 54 to 82	39.05 %	Up	pH-metric	60.7	30.5 M	0.177 M	27.1°C
11I-13010 Points 28 to 53	52.22 %	Up	pH-metric	54.9	23.2 M	0.172 M	26.4°C
11I-13010 Points 3 to 27	65.45 %	Up	pH-metric	48.9	16.3 M	0.162 M	25.3°C

Graphs



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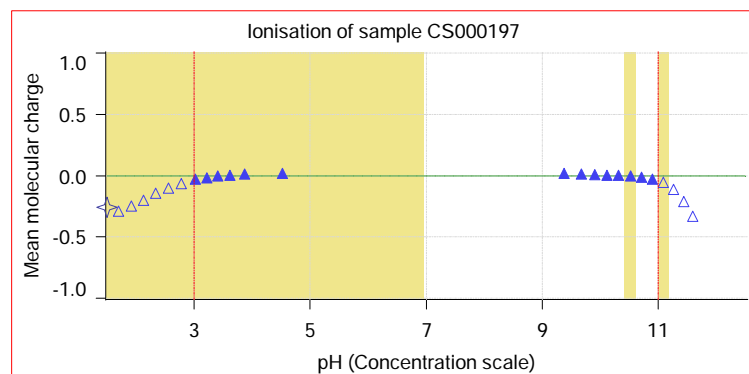
Experiment start time: **13/09/2011 16:31:36**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 1 of 3 11I-13010 Points 3 to 27

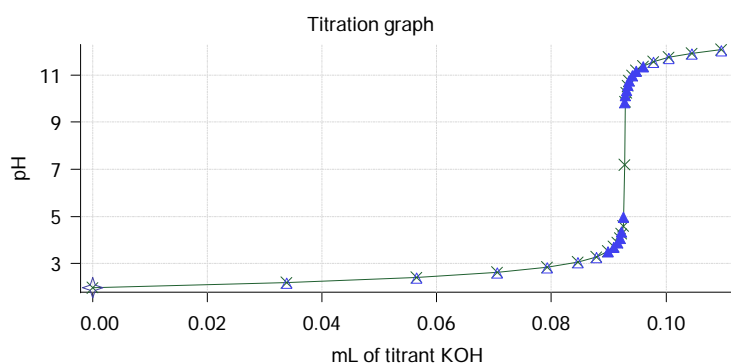
Sample

 CS000197 concentration factor 1.275

Sample graphs



Other graphs



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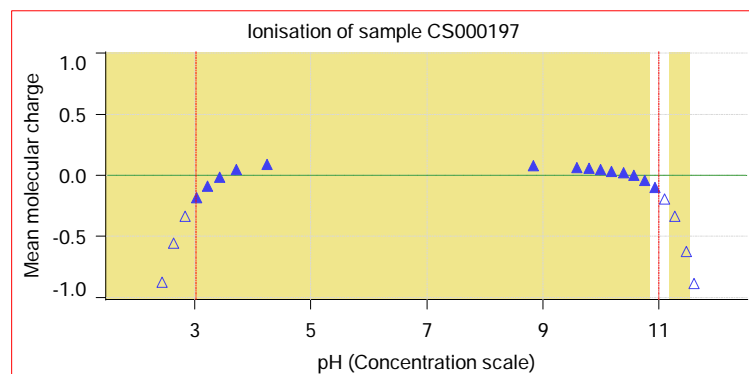
Experiment start time: **13/09/2011 16:31:36**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 2 of 3 11I-13010 Points 28 to 53

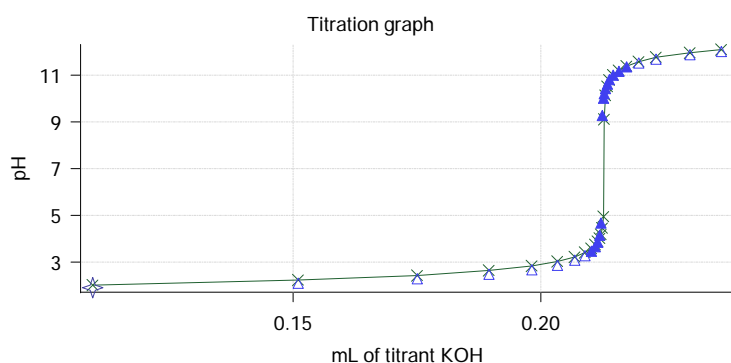
Sample

 CS000197 concentration factor 0.985

Sample graphs



Other graphs



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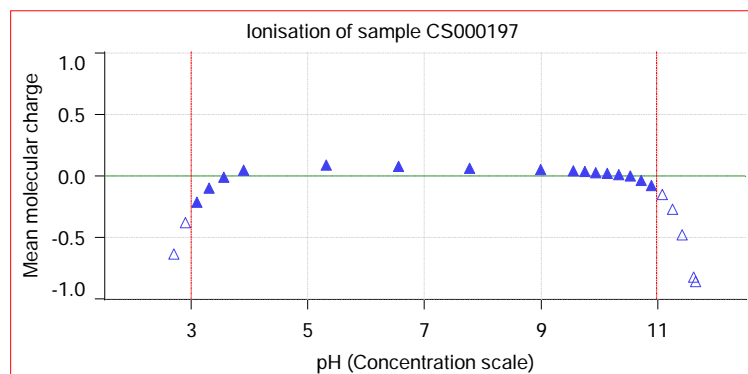
Experiment start time: **13/09/2011 16:31:36**
 Analyst:
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pH-metric psKa Titration 3 of 3 11I-13010 Points 54 to 82

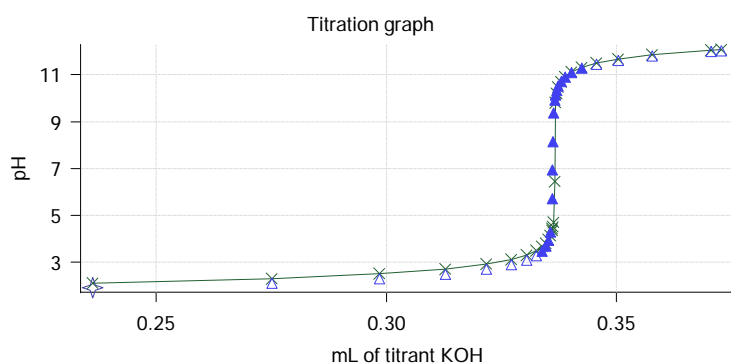
Sample

 CS000197 concentration factor 1.199

Sample graphs



Other graphs



Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000197		
Sample by	Weight		
Sample weight	0.000980 g		
Formula weight	387.49 g/mol		
Solubility	Unknown		
Molecular weight	387.49		
Individual pKa ionic environments	No		
Number of pKas	0		
logP (neutral X)	-10.00		