



Yasuda-Shedlovsky Result

Sample name: **CS000197**
Assay name: **pH-metric psKa**
Assay ID: **11I-13018**
Filename: **E:\T3 DATA\1109\11I-13018_CS000197_pH-metric psKa.t3r**

Experiment start time: **13/09/2011 21:13:21**
Analyst:
Instrument ID: **T311042**

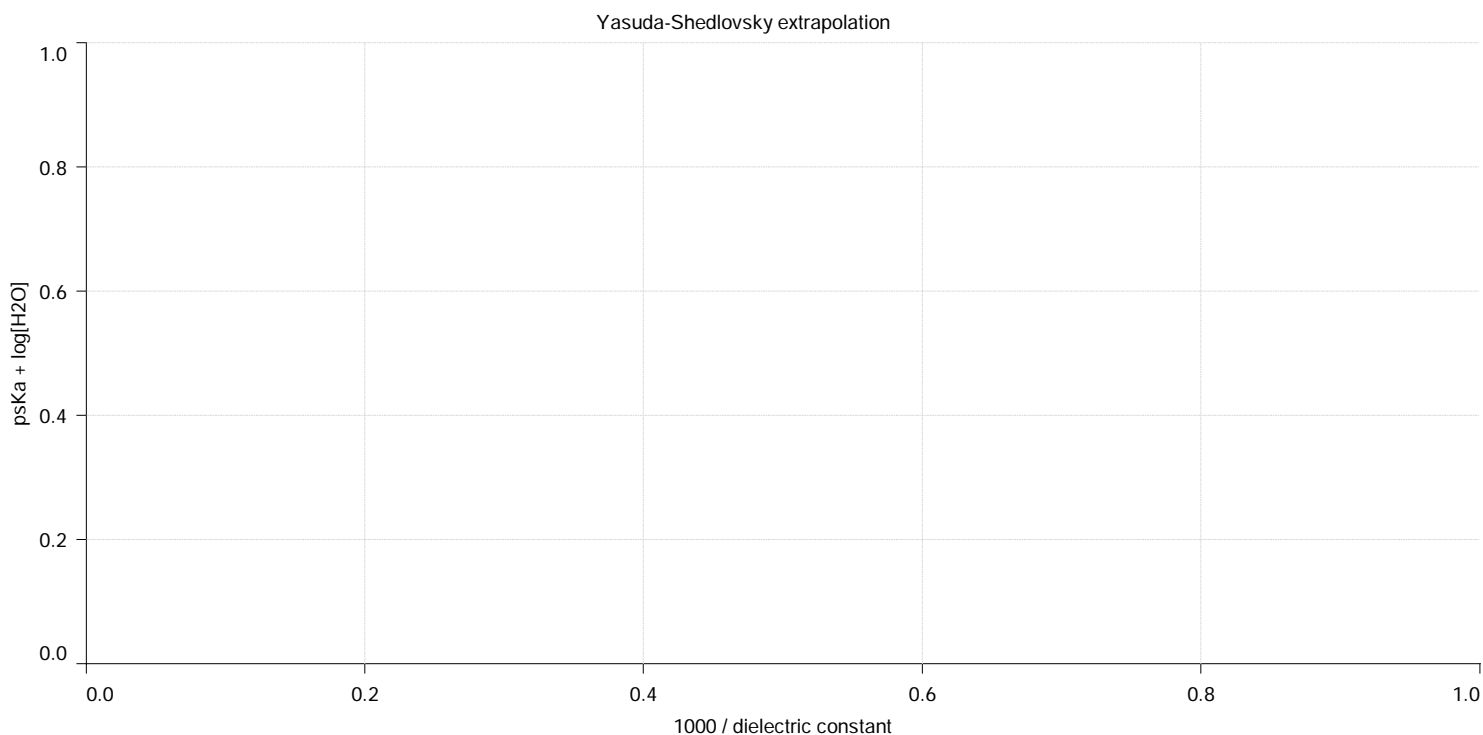
Yasuda-Shedlovsky result

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-13018 Points 58 to 94	23.02 %	Up	pH-metric	76.4	43.5 M	0.189 M	27.7°C
11I-13018 Points 28 to 57	30.10 %	Up	pH-metric	76.1	39.7 M	0.183 M	27.5°C
11I-13018 Points 3 to 27	38.55 %	Up	pH-metric	75.7	35.2 M	0.171 M	26.5°C

Graphs




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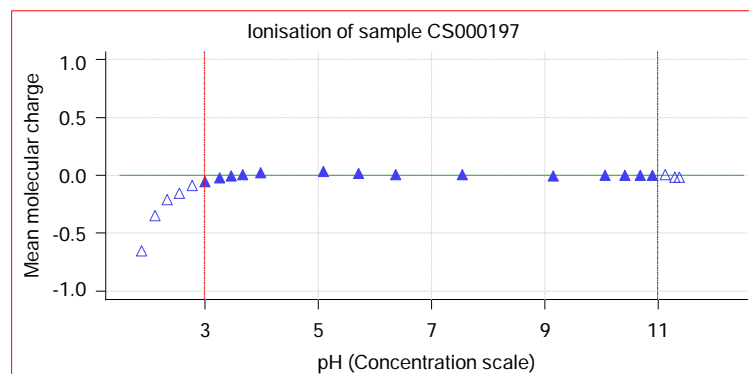
Experiment start time: **13/09/2011 21:13:21**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 1 of 3 11I-13018 Points 3 to 27

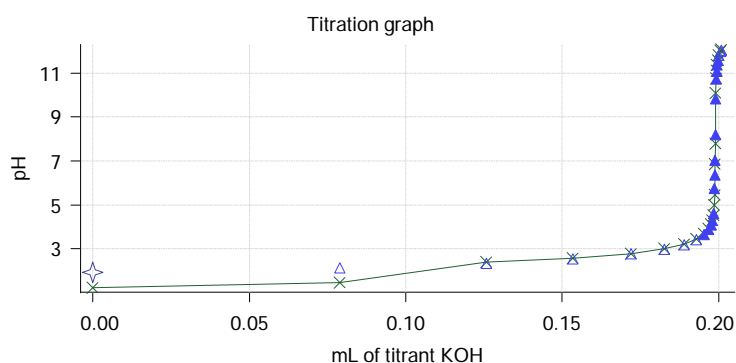
Sample

 CS000197 concentration factor 0.921

Sample graphs



Other graphs




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 Filename: **E:\T3 DATA\1109\11I-13018_CS000197_pH-metric psKa.t3r**

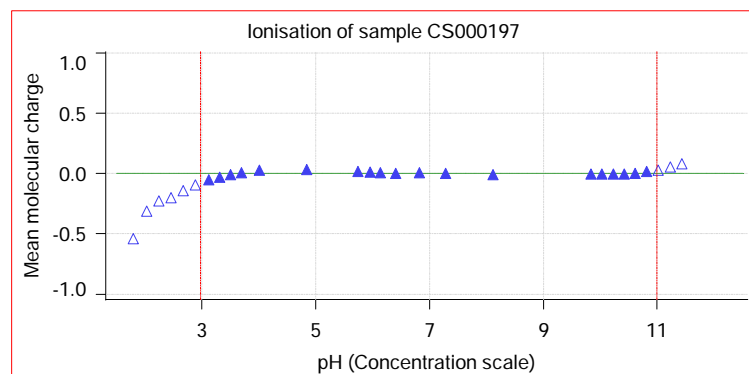
Experiment start time: **13/09/2011 21:13:21**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 2 of 3 11I-13018 Points 28 to 57

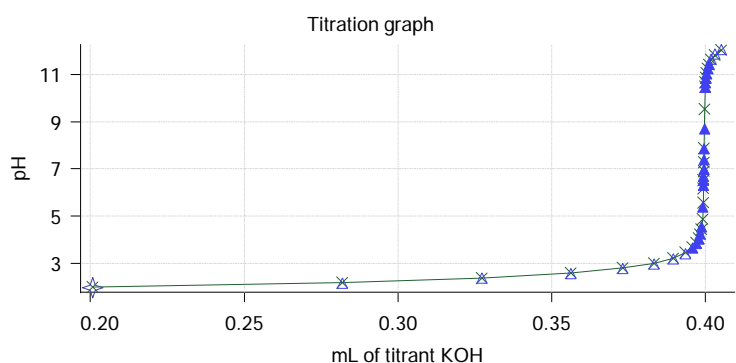
Sample

 CS000197 concentration factor 0.911

Sample graphs



Other graphs



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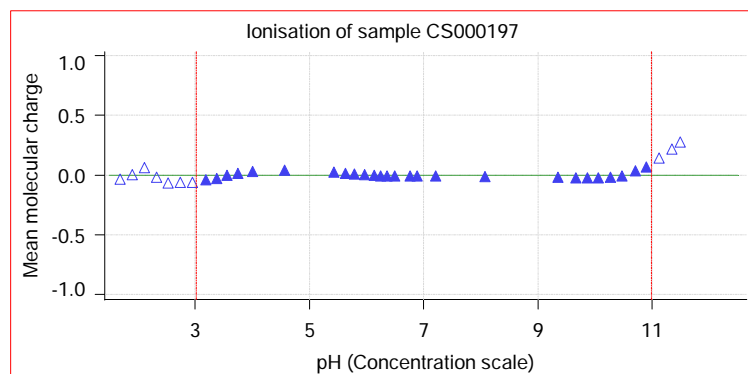
Experiment start time: **13/09/2011 21:13:21**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 3 of 3 11I-13018 Points 58 to 94

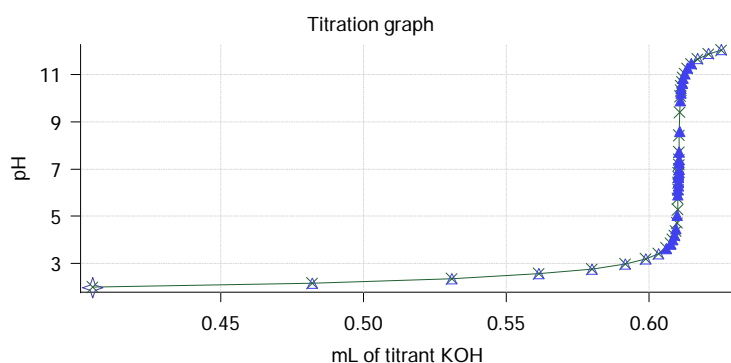
Sample

 CS000197 concentration factor 0.961

Sample graphs



Other graphs



Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000197		
Sample by	Weight		
Sample weight	0.001020 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		