



Yasuda-Shedlovsky Result

Sample name: **CS000198**
Assay name: **pH-metric psKa**
Assay ID: **11I-13011**
Filename: **E:\T3 DATA\1109\11I-13011_CS000198_pH-metric psKa.t3r**

Experiment start time: **13/09/2011 17:12:29**
Analyst:
Instrument ID: **T311042**

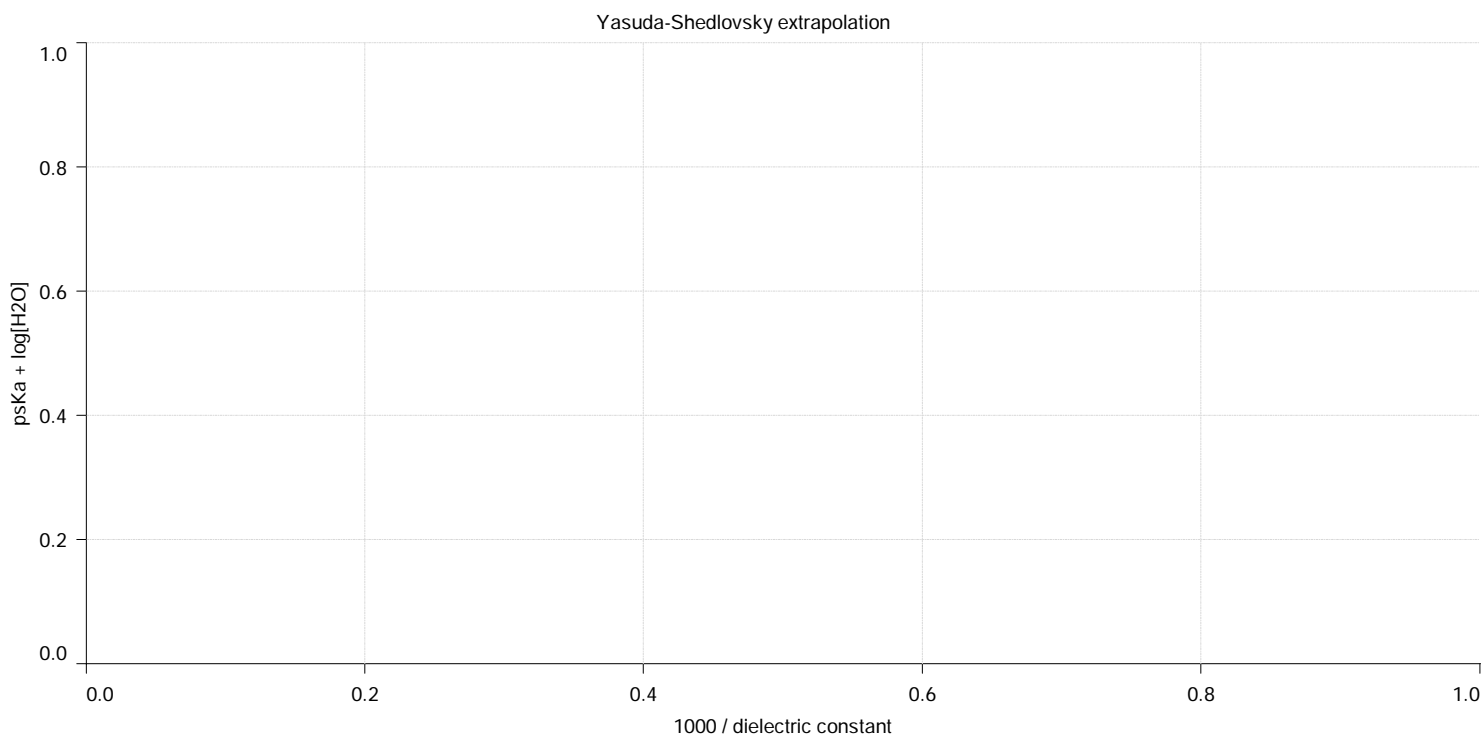
Yasuda-Shedlovsky result

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-13011 Points 54 to 78	38.59 %	Up	pH-metric	60.8	30.8 M	0.178 M	27.6°C
11I-13011 Points 28 to 53	51.57 %	Up	pH-metric	55.1	23.5 M	0.173 M	26.6°C
11I-13011 Points 3 to 27	64.58 %	Up	pH-metric	49.3	16.7 M	0.163 M	25.5°C

Graphs



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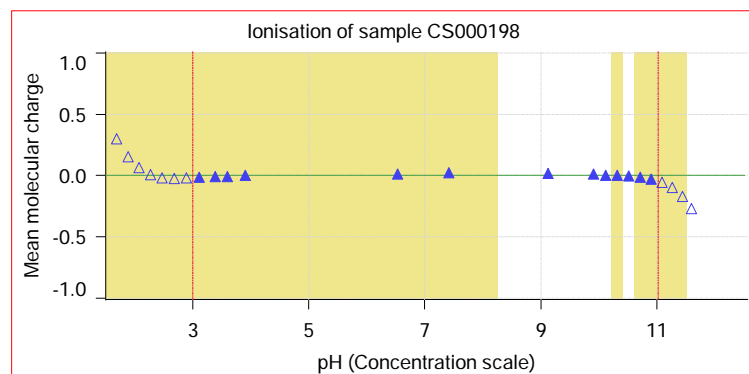
Experiment start time: **13/09/2011 17:12:29**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 1 of 3 11I-13011 Points 3 to 27

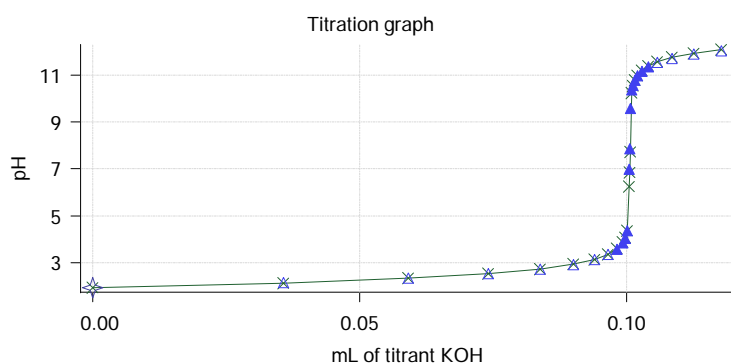
Sample

 CS000198 concentration factor 0.855

Sample graphs



Other graphs




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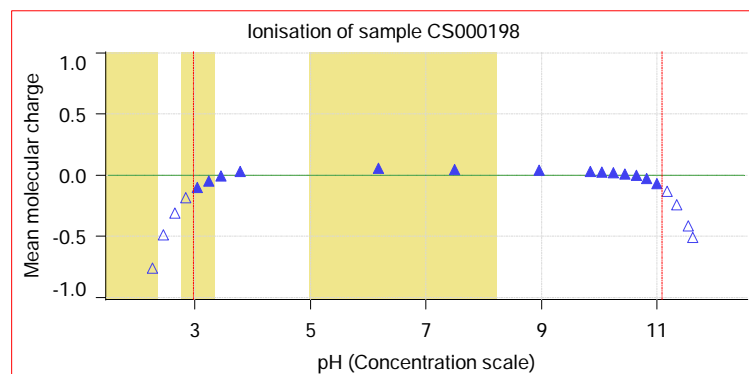
Experiment start time: **13/09/2011 17:12:29**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 2 of 3 11I-13011 Points 28 to 53

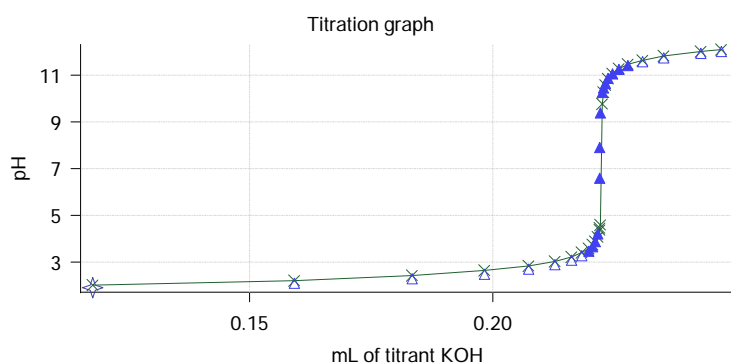
Sample

 CS000198 concentration factor 0.951

Sample graphs



Other graphs



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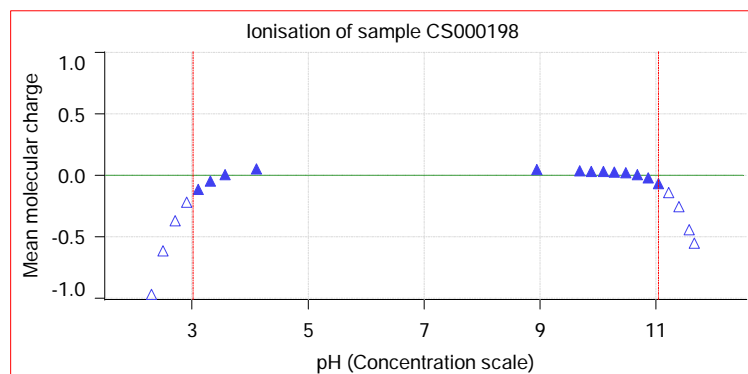
Experiment start time: **13/09/2011 17:12:29**
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pH-metric psKa Titration 3 of 3 11I-13011 Points 54 to 78

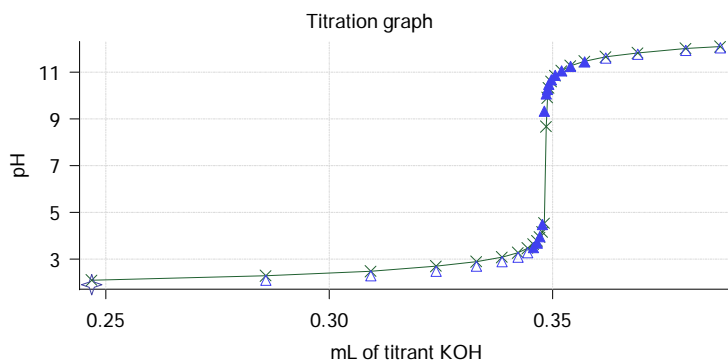
Sample

 CS000198 concentration factor 1.137

Sample graphs



Other graphs



Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000198		
Sample by	Weight		
Sample weight	0.001170 g		
Formula weight	278.33 g/mol		
Solubility	Unknown		
Molecular weight	278.33		
Individual pKa ionic environments	No		
Number of pKas	0		
logP (neutral X)	-10.00		