

Sample name: **cs000275**
 Assay name: **pH-metric psKa**
 Assay ID: **11H-31006**
 Filename: **E:\T3 DATA\1108\11H-31006_cs000275_pH-metric psKa.t3r**

Experiment start time: **31/08/2011 11:56:18**
 Analyst:
 Instrument ID: **T311042**

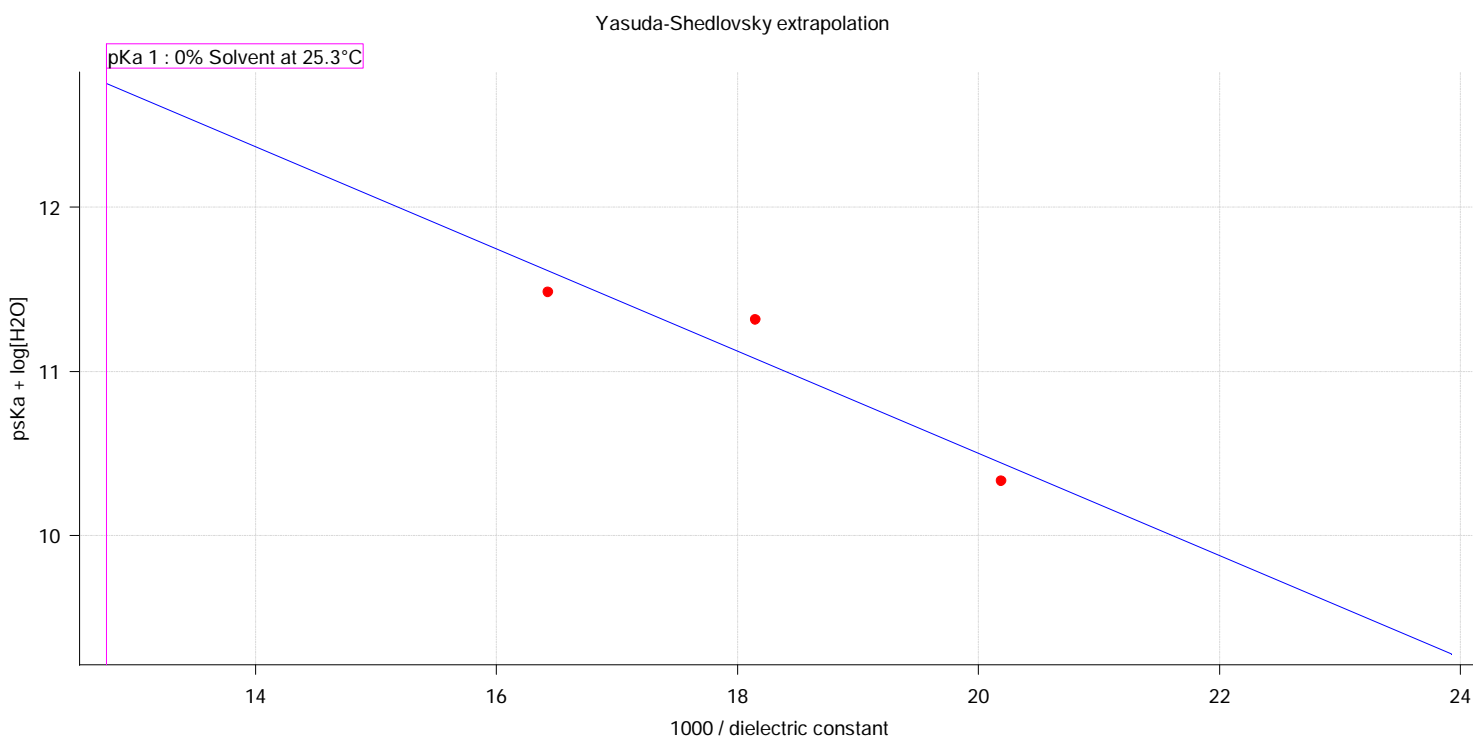
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	11.01	±0.63	16.72	-310.9860	0.8887	0.172 M	25.3°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H ₂ O]	Ionic strength	Temperature	psKa 1
11H-31006 Points 70 to 106	39.39 %	Up	pH-metric	60.9	30.3 M	0.179 M	26.2°C	✓ 10.00
11H-31006 Points 36 to 69	52.39 %	Up	pH-metric	55.1	23.1 M	0.174 M	25.4°C	✓ 9.95
11H-31006 Points 3 to 35	64.80 %	Up	pH-metric	49.5	16.6 M	0.164 M	24.3°C	✓ 9.11

Graphs





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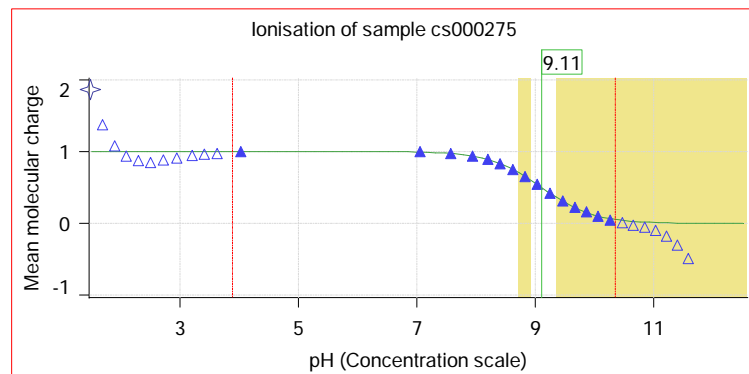
Experiment start time: **31/08/2011 11:56:18**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 1 of 3 11H-31006 Points 3 to 35

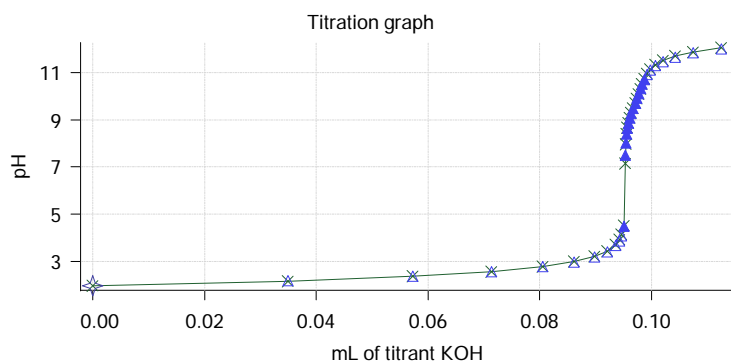
Sample

 cs000275 concentration factor 0.605
 Base pKa 1 9.11

Sample graphs



Other graphs





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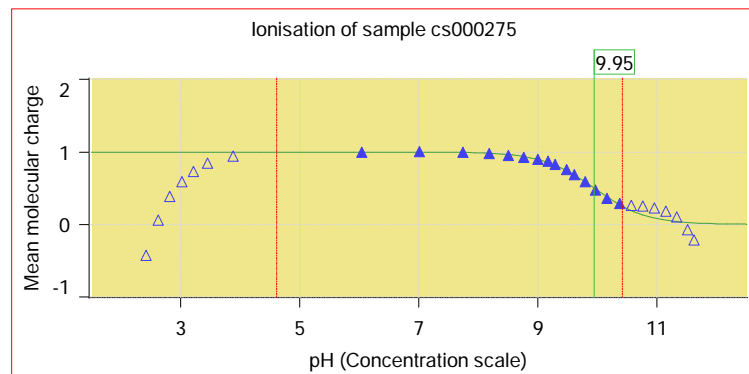
Experiment start time: **31/08/2011 11:56:18**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 2 of 3 11H-31006 Points 36 to 69

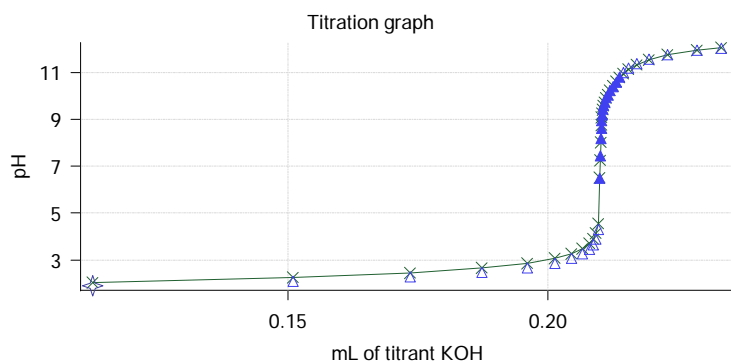
Sample

 cs000275 concentration factor 0.779
 Base pKa 1 9.95

Sample graphs



Other graphs



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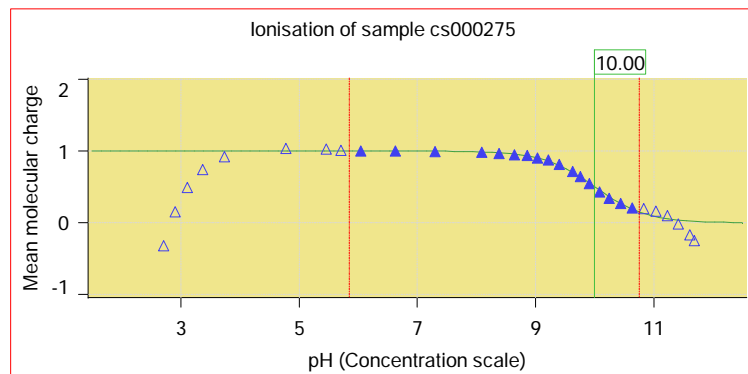
Experiment start time: **31/08/2011 11:56:18**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 3 of 3 11H-31006 Points 70 to 106

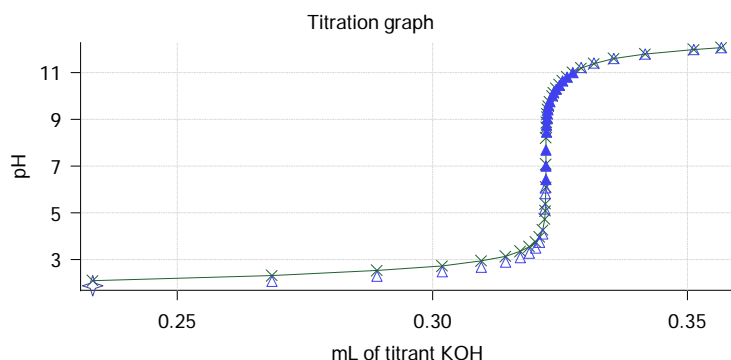
Sample

cs000275 concentration factor 0.695
 Base pKa 1 10.00

Sample graphs



Other graphs



Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	cs000275		
Sample by	Weight	31/08/2011 10:24:46	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Sample weight	0.000810 g		
Formula weight	340.71 g/mol		
Solubility	Unknown	31/08/2011 10:24:46	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	340.71		
Individual pKa ionic environments	No		
Number of pKas	1	31/08/2011 10:24:46	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Sample is a	Base	31/08/2011 10:24:46	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	4.00	31/08/2011 10:24:46	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r



Assay model

Sample name: **cs000275** Experiment start time: **31/08/2011 11:56:18**
Assay name: **pH-metric psKa** Analyst:
Assay ID: **11H-31006** Instrument ID: **T311042**
Filename: **E:\T3 DATA\1108\11H-31006_cs000275_pH-metric psKa.t3r**

Assay Model (continued)

Settings	Value	Date/Time changed	Imported from
logp (XH +)	-10.00	31/08/2011 10:24:46	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logP (neutral X)	-10.00	31/08/2011 10:24:46	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
