



Yasuda-Shedlovsky Result

Sample name: **CS000243**
Assay name: **pH-metric psKa**
Assay ID: **11H-30013**
Filename: **E:\T3 DATA\1108\11H-30013_CS000243_pH-metric psKa.t3r**

Experiment start time: **30/08/2011 18:18:44**
Analyst:
Instrument ID: **T311042**

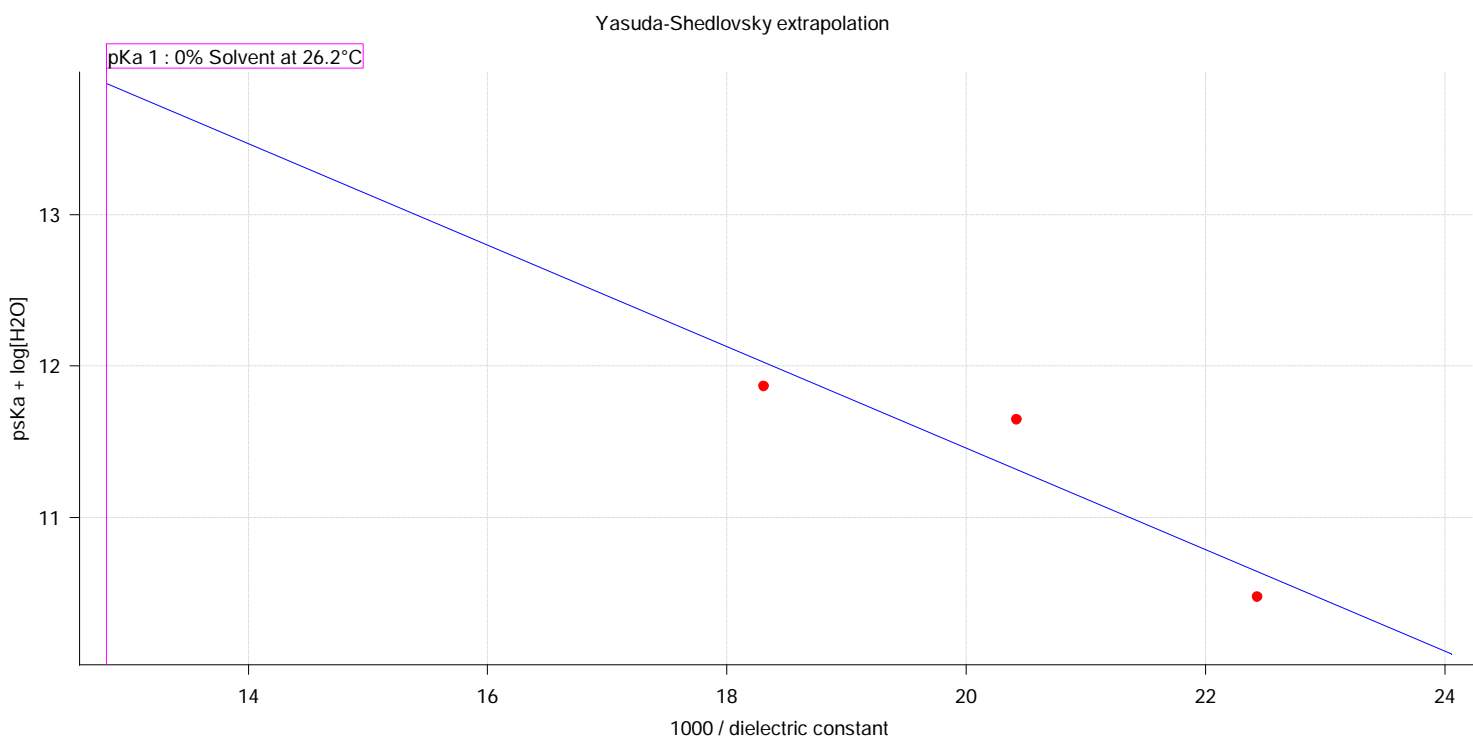
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	12.12	±1.07	18.16	-335.1102	0.8557	0.154 M	26.2°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H ₂ O]	Ionic strength	Temperature	psKa 1
11H-30013 Points 50 to 70	52.31 %	Up	pH-metric	54.6	23.1 M	0.155 M	27.1°C	✓ 10.50
11H-30013 Points 27 to 49	64.88 %	Up	pH-metric	49.0	16.6 M	0.154 M	26.1°C	✓ 10.43
11H-30013 Points 3 to 26	74.35 %	Up	pH-metric	44.6	11.8 M	0.153 M	25.3°C	✓ 9.40

Graphs



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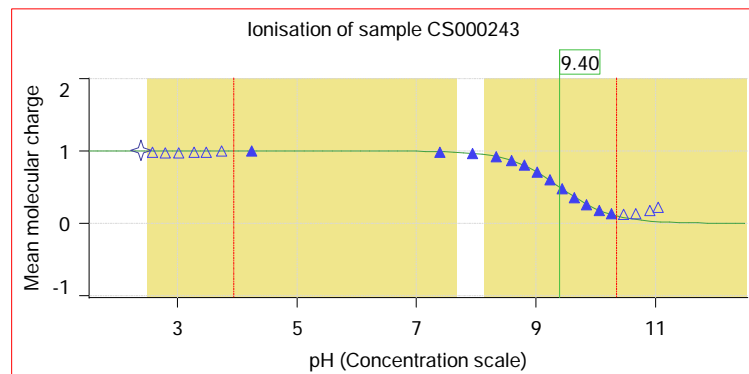
Experiment start time: **30/08/2011 18:18:44**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 1 of 3 11H-30013 Points 3 to 26

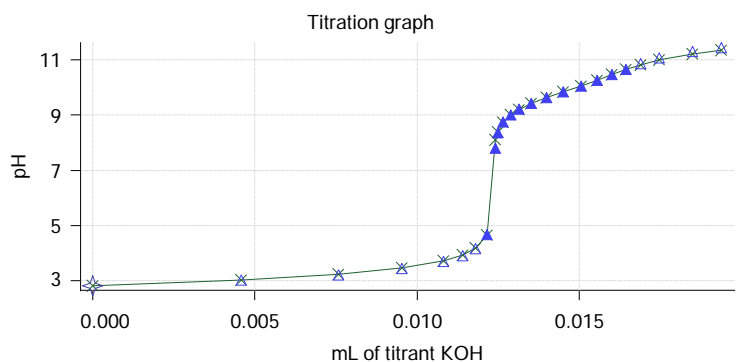
Sample

CS000243 concentration factor 0.841
 Base pKa 1 9.40

Sample graphs



Other graphs



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 Filename: **E:\T3 DATA\1108\11H-30013_CS000243_pH-metric psKa.t3r**

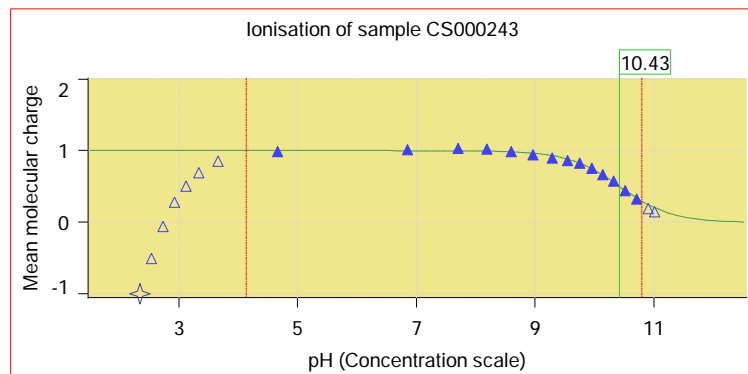
Experiment start time: **30/08/2011 18:18:44**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 2 of 3 11H-30013 Points 27 to 49

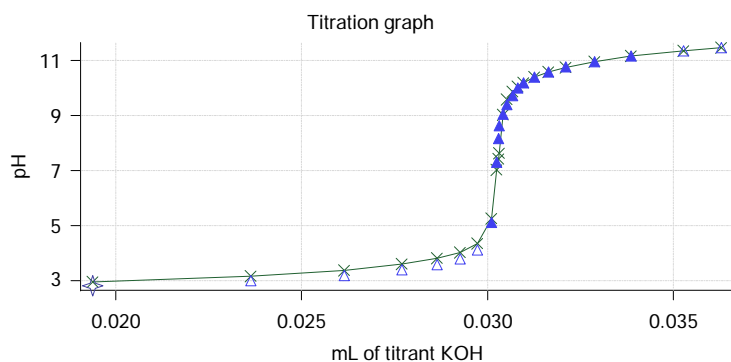
Sample

CS000243 concentration factor 0.444
 Base pKa 1 10.43

Sample graphs



Other graphs



Sample name: **CS000243**
 Assay name: **pH-metric psKa**
 Assay ID: **11H-30013**
 Filename: **E:\T3 DATA\1108\11H-30013_CS000243_pH-metric psKa.t3r**

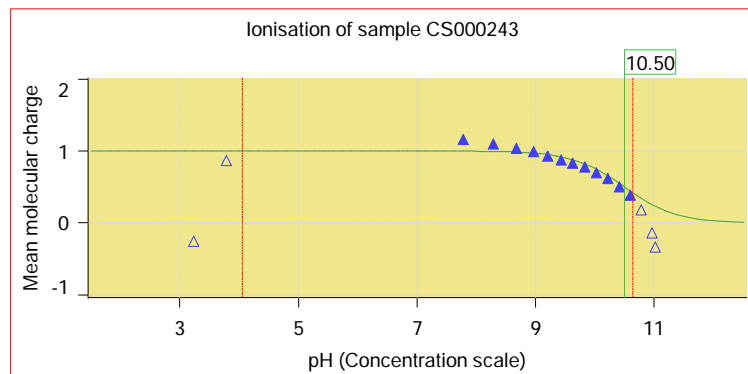
Experiment start time: **30/08/2011 18:18:44**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 3 of 3 11H-30013 Points 50 to 70 Quality: Good

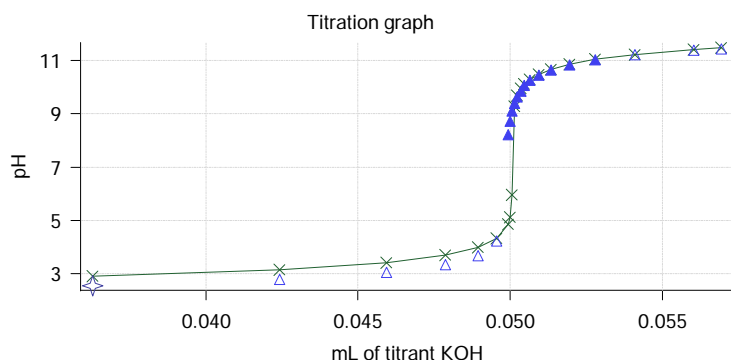
Sample

CS000243 concentration factor 0.207
 Base pKa 1 10.50

Sample graphs



Other graphs



Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000243		
Sample by	Weight		
Sample weight	0.000890 g		
Formula weight	371.39 g/mol		
Solubility	Unknown	30/08/2011 15:57:23	E:\T3 DATA\1108\11H-29005_CS000031_Fast UV psKa.t3r
Molecular weight	371.39		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base	30/08/2011 15:57:23	E:\T3 DATA\1108\11H-29005_CS000031_Fast UV psKa.t3r
pKa 1	8.00		
logp (XH +)	-10.00	30/08/2011 15:57:23	E:\T3 DATA\1108\11H-29005_CS000031_Fast UV psKa.t3r
logP (neutral X)	-10.00		