



Yasuda-Shedlovsky Result

Sample name: **CS000252**
Assay name: **pH-metric psKa**
Assay ID: **11I-01021**
Filename: **E:\T3 DATA\1109\11I-01021_CS000252_pH-metric psKa.t3r**

Experiment start time: **01/09/2011 19:19:26**
Analyst:
Instrument ID: **T311042**

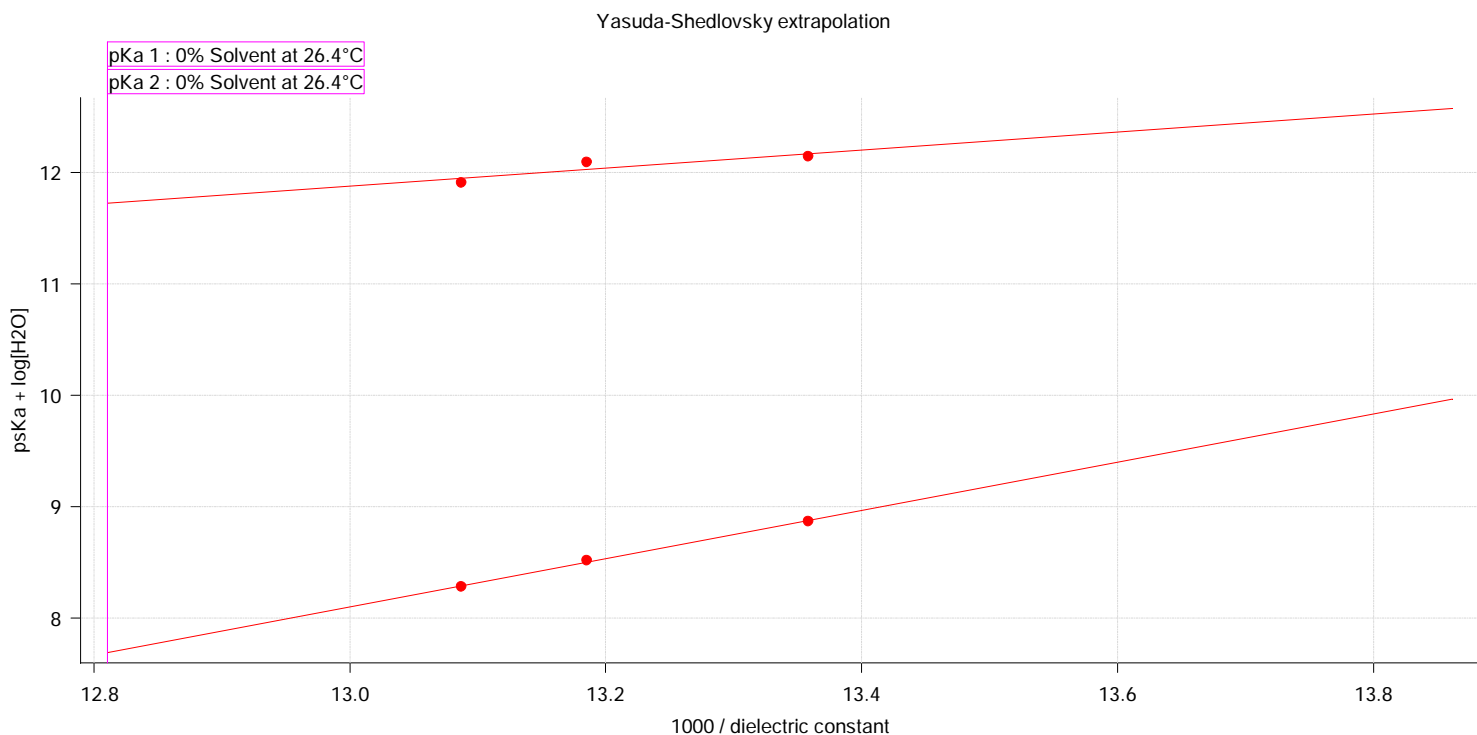
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	5.95	±0.05	-20.00	2161.5809	0.9974	0.188 M	26.4°C
Yasuda-Shedlovsky	9.98	±0.18	1.43	804.1096	0.7810	0.188 M	26.4°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature	psKa 1	sK
11I-01021 Points 105 to 157	28.65 %	Up	pH-metric	76.4	40.5 M	0.195 M	26.8°C	6.67	0.3
11I-01021 Points 54 to 104	37.27 %	Up	pH-metric	75.8	35.9 M	0.191 M	26.5°C	6.96	0.5
11I-01021 Points 3 to 53	47.23 %	Up	pH-metric	74.9	30.5 M	0.179 M	25.8°C	7.39	0.6

Graphs



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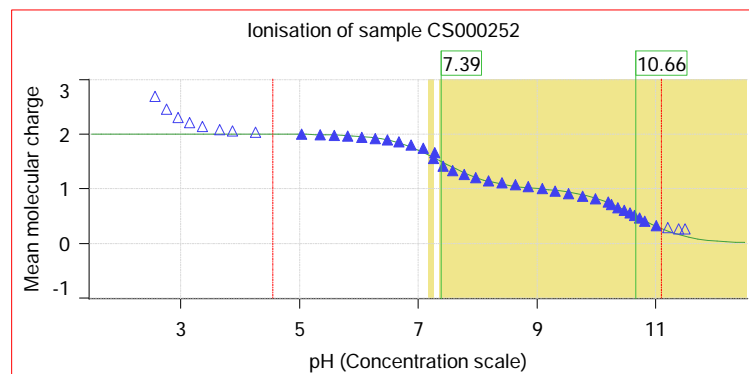
Experiment start time: **01/09/2011 19:19:26**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 1 of 3 11I-01021 Points 3 to 53

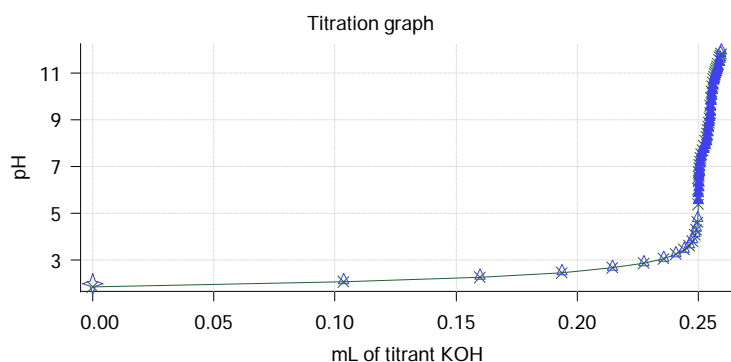
Sample

CS000252 concentration factor 0.805
 Base pKa 1 7.39
 Base pKa 2 10.66

Sample graphs



Other graphs



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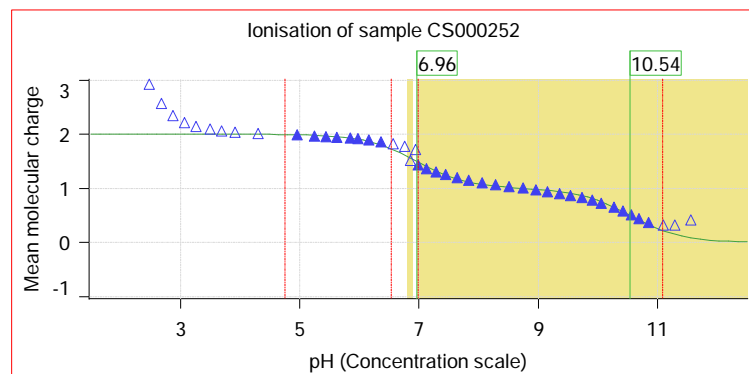
Experiment start time: **01/09/2011 19:19:26**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 2 of 3 11I-01021 Points 54 to 104

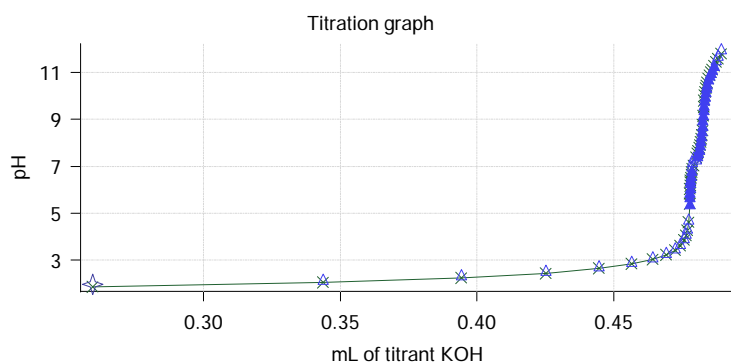
Sample

CS000252 concentration factor 0.811
 Base pKa 1 6.96
 Base pKa 2 10.54

Sample graphs



Other graphs



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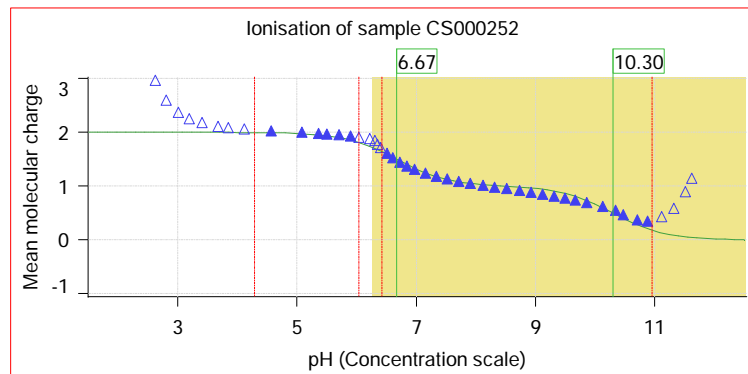
Experiment start time: **01/09/2011 19:19:26**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 3 of 3 11I-01021 Points 105 to 157 Quality: Good

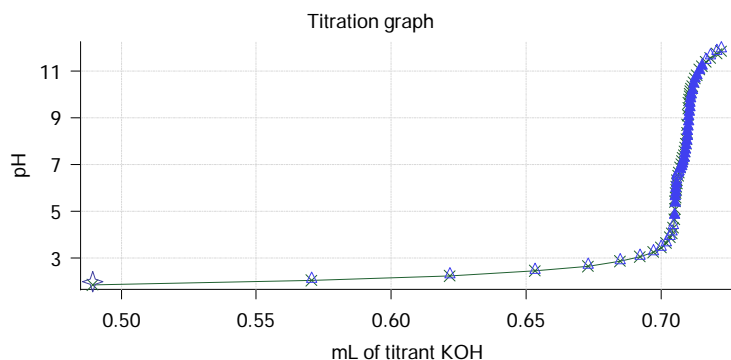
Sample

CS000252 concentration factor 0.740
 Base pKa 1 6.67
 Base pKa 2 10.30

Sample graphs



Other graphs



Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000252		
Sample by	Weight		
Sample weight	0.001090 g		
Formula weight	347.37 g/mol		
Solubility	Unknown	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
Molecular weight	347.37		
Individual pKa ionic environments	No		
Number of pKas	2		
Sample is a	Base	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
pKa 1	7.00		
pKa 2	10.30		
logP (XH2 2+)	-10.00	01/09/2011 10:40:23	E:\T3 DATA\1108\11H-01005_CS00080_pH-metric psKa.t3r
logp (XH +)	-10.00		
logP (neutral X)	-10.00		