



Yasuda-Shedlovsky Result

Sample name: **CS000270**
Assay name: **pH-metric psKa**
Assay ID: **11H-30014**
Filename: **E:\T3 DATA\1108\11H-30014_CS000270_pH-metric psKa.t3r**

Experiment start time: **30/08/2011 19:16:35**
Analyst:
Instrument ID: **T311042**

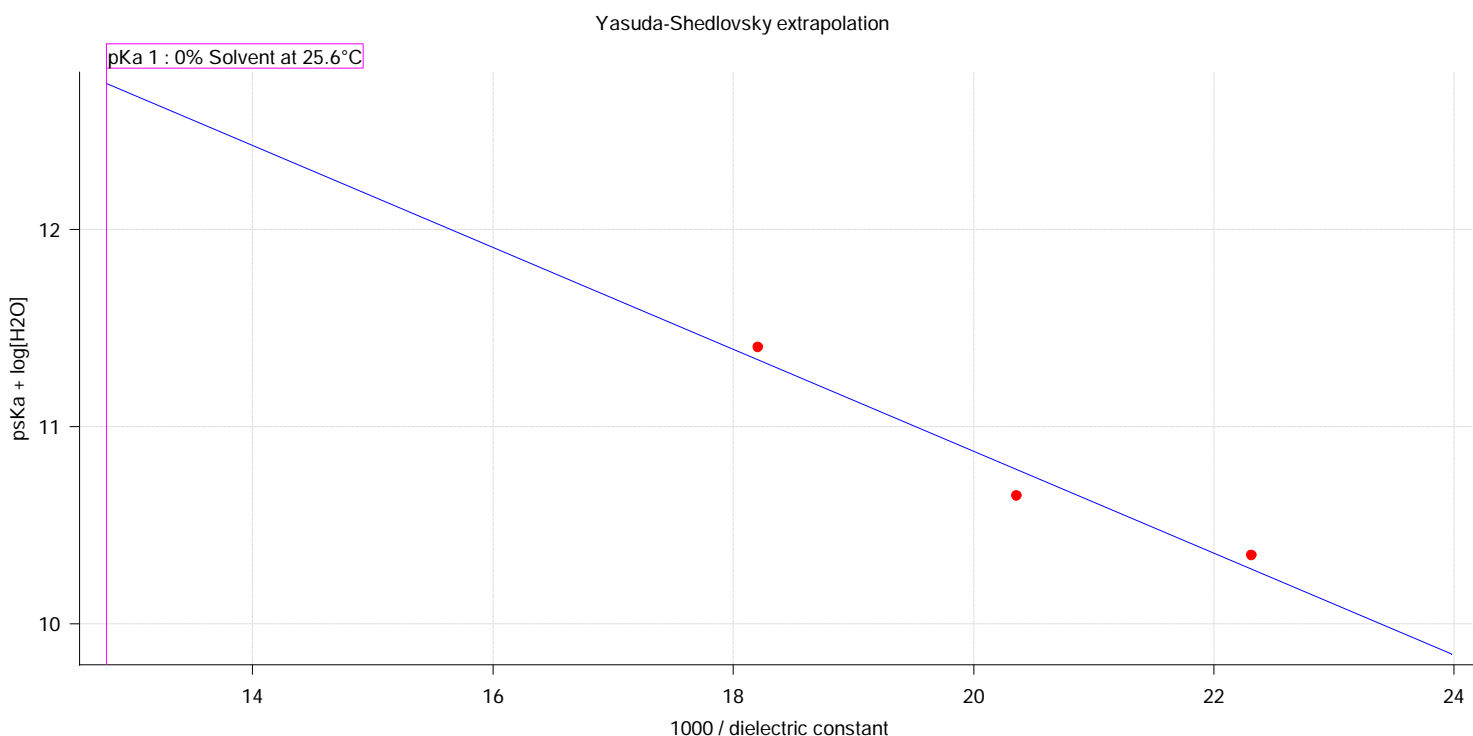
Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R ²	Ionic strength	Temperature
Yasuda-Shedlovsky	11.00	±0.43	16.04	-258.4180	0.9545	0.155 M	25.6°C

Component assay results

Titration	Methanol weight%	Direction	Result type	Dielectric constant	[H ₂ O]	Ionic strength	Temperature	psKa 1
11H-30014 Points 54 to 78	52.11 %	Up	pH-metric	54.9	23.2 M	0.157 M	26.4°C	✓ 10.04
11H-30014 Points 29 to 53	64.66 %	Up	pH-metric	49.1	16.7 M	0.155 M	25.9°C	✓ 9.43
11H-30014 Points 3 to 28	74.26 %	Up	pH-metric	44.8	11.9 M	0.153 M	24.6°C	✓ 9.27

Graphs



Sample name: **CS000270**
 Assay name: **pH-metric psKa**
 Assay ID: **11H-30014**
 Filename: **E:\T3 DATA\1108\11H-30014_CS000270_pH-metric psKa.t3r**

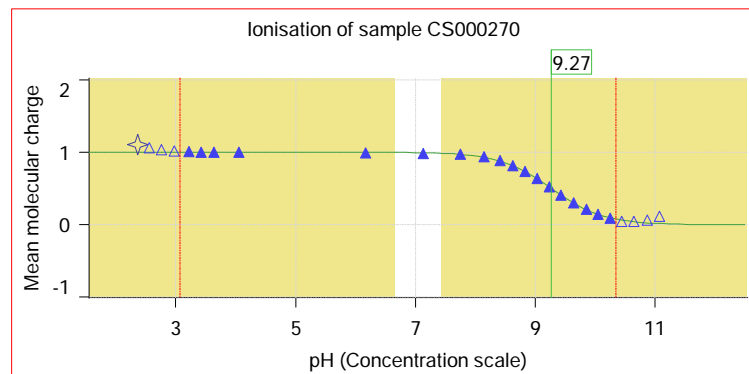
Experiment start time: **30/08/2011 19:16:35**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 1 of 3 11H-30014 Points 3 to 28

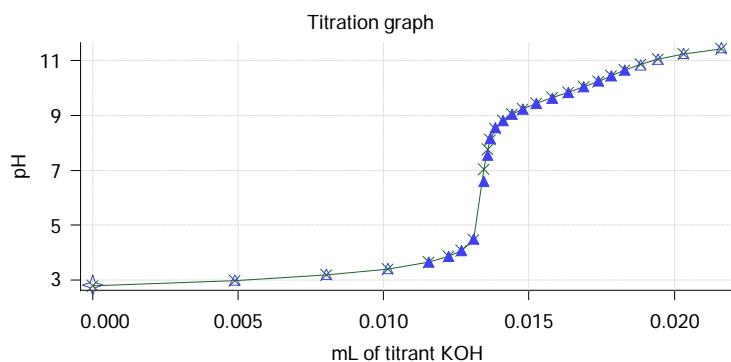
Sample

CS000270 concentration factor 0.778
 Base pKa 1 9.27

Sample graphs



Other graphs



Sample name: **CS000270**
 Assay name: **pH-metric psKa**
 Assay ID: **11H-30014**
 Filename: **E:\T3 DATA\1108\11H-30014_CS000270_pH-metric psKa.t3r**

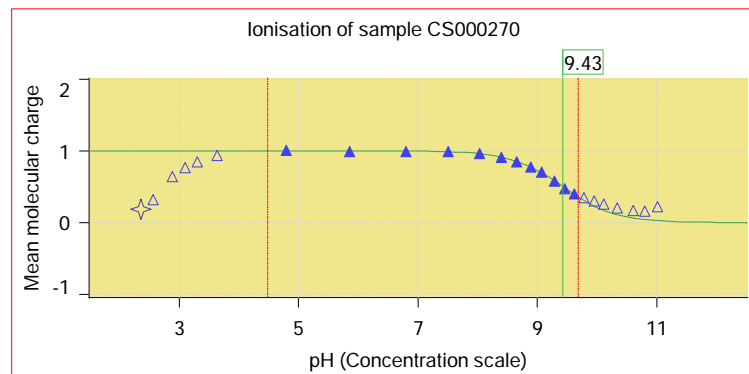
Experiment start time: **30/08/2011 19:16:35**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 2 of 3 11H-30014 Points 29 to 53

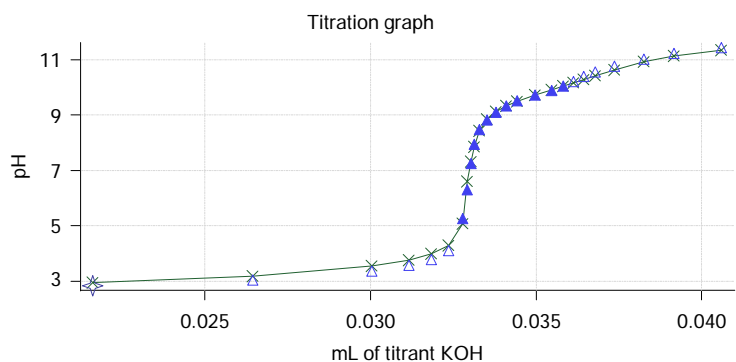
Sample

CS000270 concentration factor 0.716
 Base pKa 1 9.43

Sample graphs



Other graphs



Sample name: **CS000270**
 Assay name: **pH-metric psKa**
 Assay ID: **11H-30014**
 Filename: **E:\T3 DATA\1108\11H-30014_CS000270_pH-metric psKa.t3r**

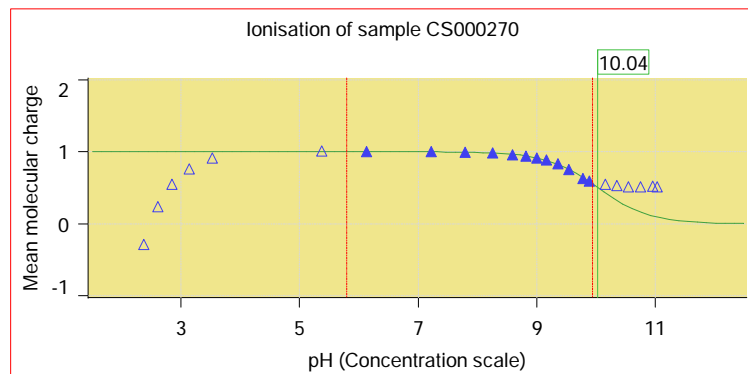
Experiment start time: **30/08/2011 19:16:35**
 Analyst:
 Instrument ID: **T311042**

pH-metric psKa Titration 3 of 3 11H-30014 Points 54 to 78

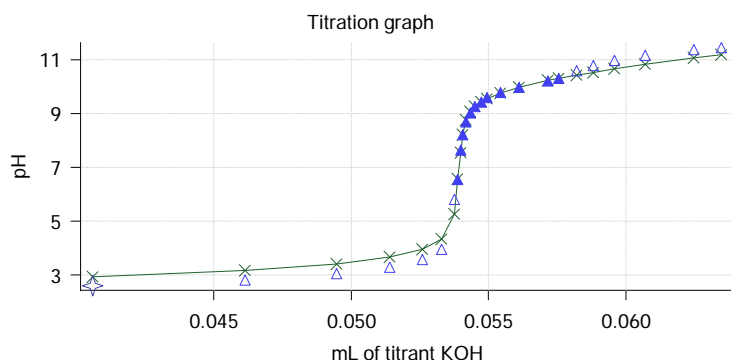
Sample

CS000270 concentration factor 1.298
 Base pKa 1 10.04

Sample graphs



Other graphs



Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000270		
Sample by	Weight		
Sample weight	0.000960 g		
Formula weight	324.64 g/mol		
Solubility	Unknown	30/08/2011 15:57:23	E:\T3 DATA\1108\11H-29005_CS000031_Fast UV psKa.t3r
Molecular weight	324.64		
Individual pKa ionic environments	No		
Number of pKas	1	30/08/2011 15:57:23	E:\T3 DATA\1108\11H-29005_CS000031_Fast UV psKa.t3r
Sample is a	Base	30/08/2011 15:57:23	E:\T3 DATA\1108\11H-29005_CS000031_Fast UV psKa.t3r
pKa 1	4.00	30/08/2011 15:57:23	E:\T3 DATA\1108\11H-29005_CS000031_Fast UV psKa.t3r
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	30/08/2011 15:57:23	E:\T3 DATA\1108\11H-29005_CS000031_Fast UV psKa.t3r