

Sample name: CS000200
Assay name: pH-metric psKa
Assay ID: 11I-14010
Filename: E:\T3 DATA\1109\11I-14010_CS000200_pH-metric psKa.t3r

Experiment start time: 14/09/2011 18:13:32
Analyst:
Instrument ID: T311042

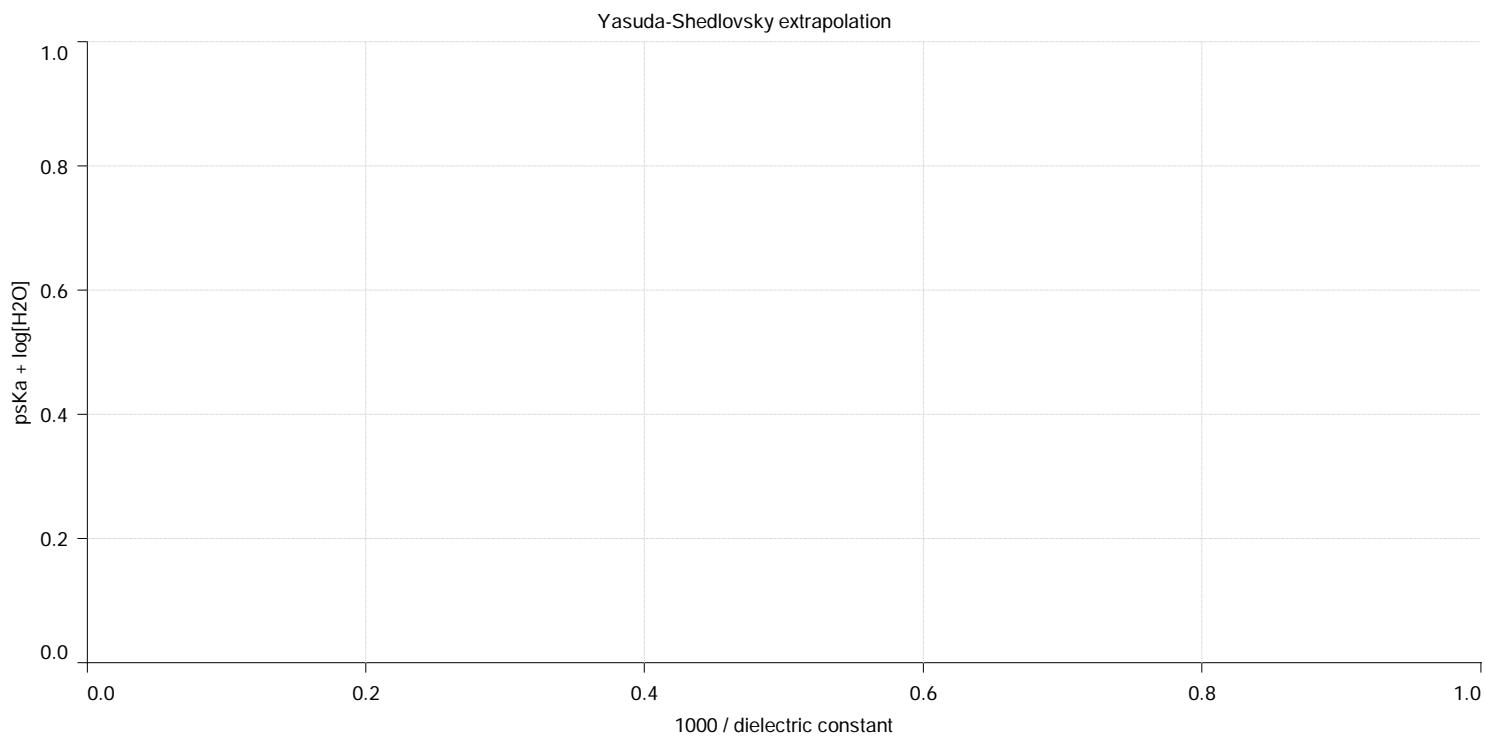
Yasuda-Shedlovsky result

Extrapolation type pKa 0% SD Intercept Slope R² Ionic strength Temperature

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H ₂ O]	Ionic strength	Temperature
11I-14010 Points 64 to 102	27.38 %	Up	pH-metric	75.8	41.1 M	0.196 M	28.8°C
11I-14010 Points 31 to 63	35.29 %	Up	pH-metric	75.3	36.9 M	0.191 M	28.5°C
11I-14010 Points 3 to 30	44.79 %	Up	pH-metric	74.5	31.8 M	0.179 M	27.8°C

Graphs



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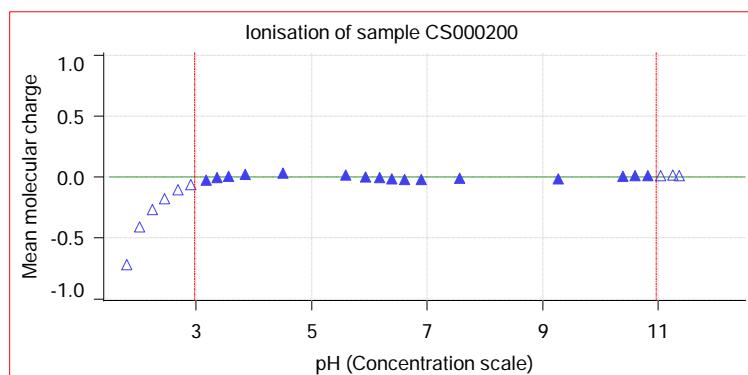
Experiment start time: 14/09/2011 18:13:32
Analyst:
Instrument ID: T311042

pH-metric psKa Titration 1 of 3 11I-14010 Points 3 to 30

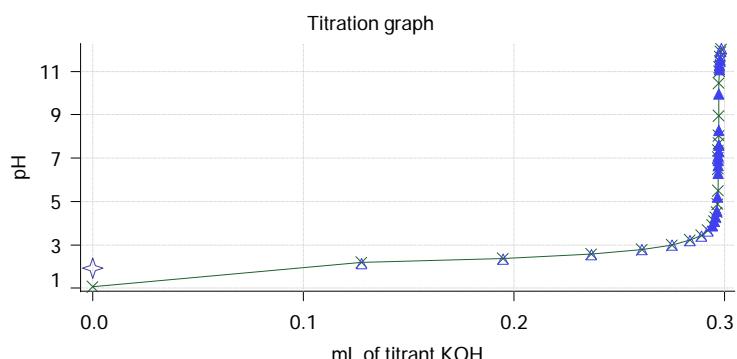
Sample

CS000200 concentration factor 0.811

Sample graphs



Other graphs



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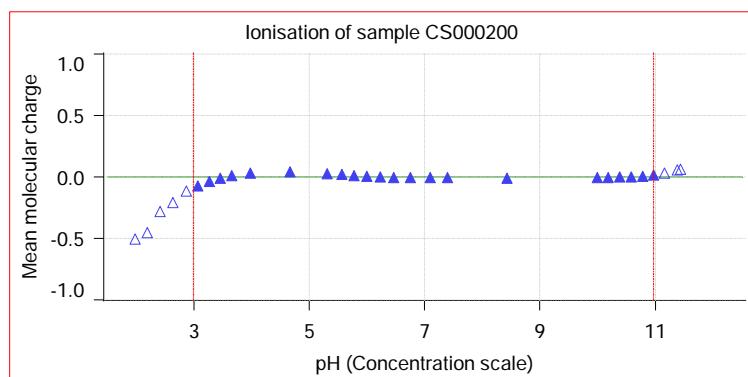
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Analyst:
Instrument ID: T311042

pH-metric psKa Titration 2 of 3 11I-14010 Points 31 to 63

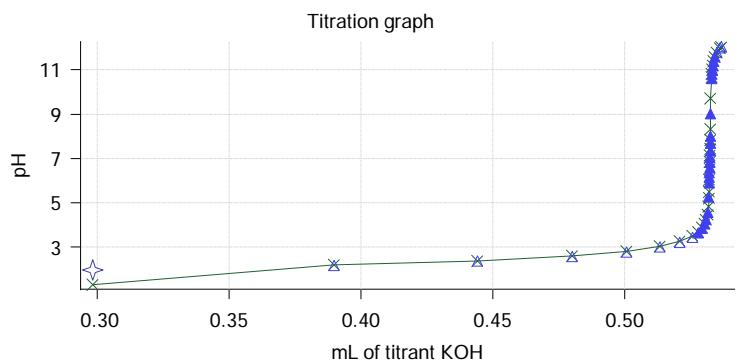
Sample

CS000200 concentration factor 0.875

Sample graphs



Other graphs



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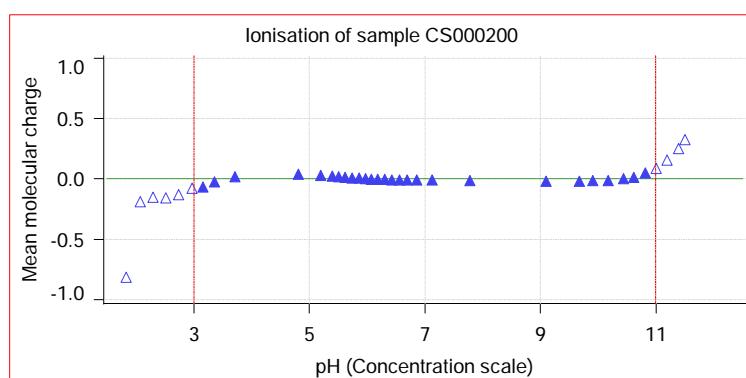
Experiment start time: 14/09/2011 18:13:32
Analyst:
Instrument ID: T311042

pH-metric psKa Titration 3 of 3 11I-14010 Points 64 to 102

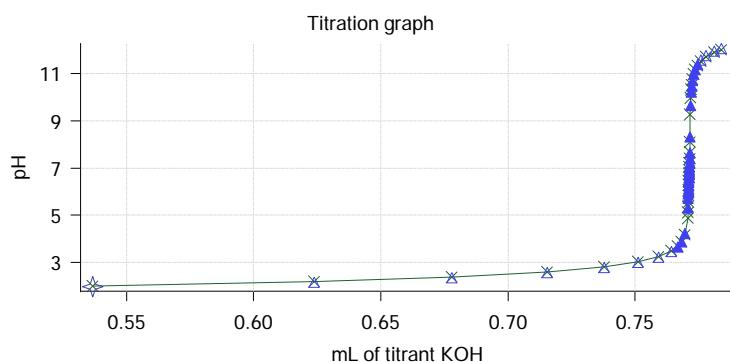
Sample

CS000200 concentration factor 0.964

Sample graphs



Other graphs



Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000200		
Sample by	Weight		
Sample weight	0.000970 g		
Formula weight	366.76 g/mol		
Solubility	Unknown		
Molecular weight	Unknown		
Individual pKa ionic environments	No		
Number of pKas	0		
logP (neutral X)	-10.00		