Yasuda-Shedlovsky Result

Sample name:	**CS000189**	Experiment start time:	**05/09/2011 15:20:23**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-05011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-05011_CS000189_pH-metric psKa.t3r**		

Yasuda-Shedlovsky result

Extrapolation type	pKa 0%	SD	Intercept	Slope	R^2	Ionic strength	Temperature
Yasuda-Shedlovsky	4.82	±0.04	25.41	-1472.6698	0.9930	0.190 M	26.1°C

Component assay results

Titration	DMSO weight%	Direction	Result type	Dielectric constant	[H2O]	Ionic strength	Temperature		psKa 1
11I-05011 Points 85 to 132	25.30 %	Up	pH-metric	76.7	42.3 M	0.197 M	26.6°C	☑	4.58
11I-05011 Points 41 to 84	33.47 %	Up	pH-metric	76.2	37.9 M	0.193 M	26.3°C	☑	4.50
11I-05011 Points 3 to 40	43.95 %	Up	pH-metric	75.4	32.3 M	0.181 M	25.4°C	☑	4.38

Graphs

Sample name:	**CS000189**	Experiment start time:	**05/09/2011 15:20:23**
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Filename:	**E:\T3 DATA\1109\11I-05011_CS000189_pH-metric psKa.t3r**		

pH-metric psKa Titration 1 of 3 11I-05011 Points 3 to 40

Sample

- CS000189 concentration factor 0.865
- Base pKa 1 4.38

Sample graphs

Other graphs

Sample name:	**CS000189**	Experiment start time:	**05/09/2011 15:20:23**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-05011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-05011_CS000189_pH-metric psKa.t3r**		

pH-metric psKa Titration 2 of 3 11I-05011 Points 41 to 84

Sample

CS000189 concentration factor	0.886
Base pKa 1	4.50

Sample graphs

Other graphs

Sample name:	**CS000189**	Experiment start time:	**05/09/2011 15:20:23**
Assay name:	**pH-metric psKa**	Analyst:	
Assay ID:	**11I-05011**	Instrument ID:	**T311042**
Filename:	**E:\T3 DATA\1109\11I-05011_CS000189_pH-metric psKa.t3r**		

pH-metric psKa Titration 3 of 3 11I-05011 Points 85 to 132

Sample

CS000189 concentration factor	0.908
Base pKa 1	4.58

Sample graphs

Other graphs

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	CS000189		
Sample by	Weight		
Sample weight	0.001070 g		
Formula weight	295.30 g/mol		
Solubility	Unknown		
Molecular weight	295.30		
Individual pKa ionic environments	No		
Number of pKas	1		
Sample is a	Base		
pKa 1	2.69		
logp (XH +)	-10.00		
logP (neutral X)	-10.00		